Supplementary Information

S1 Modified Stern–Volmer equation

$$\frac{F_0}{F_0 - F} = \frac{1}{f_a K_{sv}} \frac{1}{[\mathrm{Q}]} + \frac{1}{f_a} \quad \text{(S1)}$$

F_0 and F are the relative fluorescence intensities of CAT in the absence and presence of the Hg(II), respectively; f_a is the fraction of fluorophore accessible to the quencher; [Q] is the concentration of Hg(II), and K_{sv} is the modified Stern–Volmer quenching constant.

S2 Double logarithm equation

$$\log \frac{F_0 - F}{F} = \log K + n \log[\mathrm{Q}] \quad \text{(S2)}$$

K_b is the binding constant for the Hg(II)-CAT interaction and n is the number of binding sites per CAT molecule, which can be determined by the slope and the intercept of the double logarithm regression curve of log((*F*$_0$-*F*) /*F*) versus log [*Q*].

S3 Van't Hoff equation and thermodynamic equation

$$\ln K = -\Delta H / \mathrm{R}\, T + \Delta S / \mathrm{R} \quad \text{(S3)}$$

$$\Delta G = \Delta H - T\Delta S \quad \text{(S4)}$$

K is the binding constant at temperature T and R is the universal gas constant.

S4 The species of Hg(II) in the experimental system

The coordination reactions of Hg(II) with Cl^- in the experimental system mainly follow equations S5-S8:

$$Hg^{2+} + Cl^- \; \mathfrak{f} \; [\mathrm{HgCl}]^+ \; \beta_1 = 10^{6.74} \quad \text{(S5)}$$

$$Hg^{2+} + 2Cl^- \; \mathfrak{f} \; \mathrm{HgCl_2^0} \; \beta_2 = 10^{13.22} \quad \text{(S6)}$$

$$Hg^{2+} + 3Cl^- \rightleftharpoons [HgCl_3]^- \quad \beta_3 = 10^{14.07} \tag{S7}$$

$$Hg^{2+} + 4Cl^- \rightleftharpoons [HgCl_4]^{2-} \quad \beta_4 = 10^{15.07} \tag{S8}$$

Meanwhile, the experimental system can undergo coordination equilibriums of Hg(II) with OH^- in these ways (equations S9-S11):

$$Hg^{2+} + OH^- \rightleftharpoons [HgOH]^+ \quad \beta_1' = 10^{10.6} \tag{S9}$$

$$Hg^{2+} + 2OH^- \rightleftharpoons Hg(OH)_2^0 \quad \beta_2' = 10^{21.8} \tag{S10}$$

$$Hg^{2+} + 3OH^- \rightleftharpoons [Hg(OH)_3]^- \quad \beta_3' = 10^{20.9} \tag{S11}$$

where β stands for the stability constants of the complexes. Then, the equilibrium equation was obtained from equation S12:

$$\begin{aligned} C_{Hg(II)} = [Hg^{2+}]\{1 + \beta_1[Cl^-] + \beta_2[Cl^-]^2 + \beta_3[Cl^-]^3 + \beta_4[Cl^-]^4 \\ + \beta_1'[OH^-] + \beta_2'[OH^-]^2 + \beta_3'[OH^-]^3\} \end{aligned} \tag{S12}$$

The distribution fractions (ψ_x) of different species of Hg(II) can be calculated from equation S13:

$$\psi_X = C_X / C_{Hg(II)} \tag{S13}$$

where x=Hg^{2+}, $[HgCl]^+$, $HgCl_2$, $[HgCl_3]^-$, $[HgCl_4]^{2-}$, $[HgOH]^+$, $Hg(OH)_2$, $[Hg(OH)_3]^-$, successively.

As the pH value of the buffer solution is 7.40, $[OH^-]$ in our experimental system is $10^{-6.6}$ mol L^{-1}. $[Cl^-]$ is equal to 0.10 mol L^{-1}, which is mainly from the buffer solution, and the contribution from dissolved $HgCl_2$ is negligible. The distribution fractions of different species of Hg(II) were calculated using the equations above, and the results are shown in Table S1.

Table S1 The distribution fractions of different species of Hg(II)

Species	Hg^{2+}	$[HgCl]^{+}$	$HgCl_2$	$[HgCl_3]^{-}$
Fraction (%)	2.49×10^{-10}	1.37×10^{-4}	41.35	29.27
Species	$[HgCl_4]^{2-}$	$[HgOH]^{+}$	$Hg(OH)_2$	$[Hg(OH)_3]^{-}$
Fraction (%)	29.27	2.49×10^{-6}	0.0991	3.14×10^{-9}