Electronic Supplementary Material (ESI) for Analytical Methods.

Supplementary Information

Polymer Capped CdSe/ZnS Quantum Dots for the Sensitive Detection of Cu^{2+} and Hg^{2+} and the Quenching Mechanism

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Preparation of CdSe QDs

TOP-Se solution was created by mixing 0.33 g Se with 2.5 mL paraffin liquid and 2.5 mL TOP and dispersed by ultrasonic. Under an nitrogen atmosphere, 0.46 g SA, 0.052 g CdO, and 5 mL liquid paraffin were transferred to a 3-neck round bottom flask. Heat the mixture under stirring to 200 °C to obtain a yellow optically clear solution. Then, the mixed solution was cooled to room temperature and 1 g TOPO, 3 g ODA, 15 mL liquid paraffin was added. Heat the solution again to 280 °C and inject 2.5 mL TOP-Se solution at a time. The reaction was stopped after 45 min, and the mixture was centrifuged and purified by acetone, n-hexane, methanol and chloroform.

Preparation of CdSe/ZnS QDs:

1. Zinc precursor solution: 0.081 g ZnO, 2.8 mL OA and 7.2 mL ODE were added to the flask in nitrogen atmosphere and heated to 300 °C until the solution was completely clear. Keep the final solution at 80 °C until the growth shell procedure is complete.

2. Sulfur precursor solution: Under an nitrogen atmosphere, 0.032 g S and 10 mL ODE were added to the flask and heated to 180 ℃ until the solution was completely clear. The temperature of the solution was cooled to room temperature and sealed away from light.

3. ZnS shell growth: 6 mL ODE, 2 g ODA and 1 g TOPO were added into the 3-neck flask. Heat the flask under an nitrogen atmosphere at 100 °C for 1 h and then cool to room temperature. Place the chloroform suspension containing the CdSe QDs in the flask and remove the chloroform and other volatiles by heating in nitrogen at 100 °C for 1 h. Then, the solution was heated to 220 °C. To calculate the amount of Zn- and S-precursor for the growth of each shell according to the literature. The precursors needed for each layer were injected into the flask at one time. After the final injection, incubate the reaction mixture for 30 min at 220 °C. Cool the reaction to room temperature and added ethanol. Transfer to centrifuge tube and 5000 r/min centrifuged 10 min. Dissolve the precipitate in hexane, add proper amount of acetone, and centrifuge 10min with 5000 r/min.

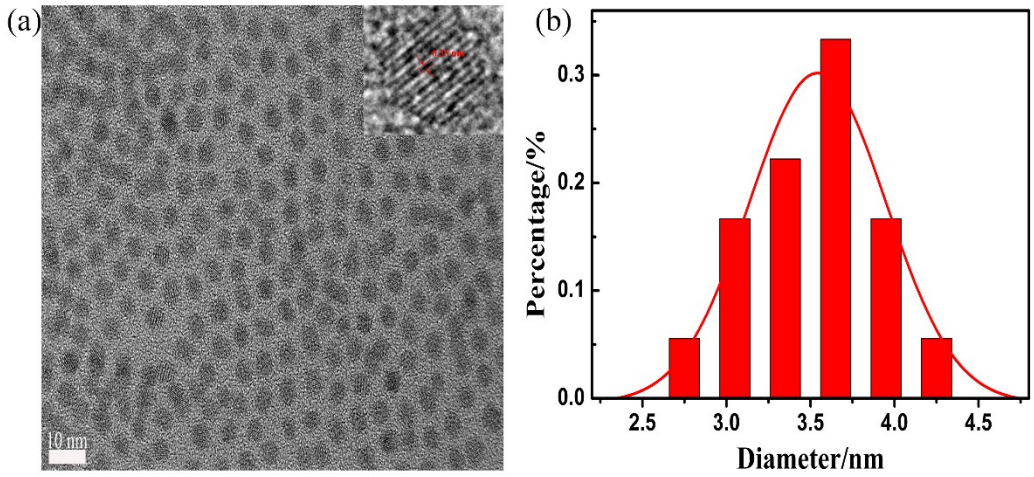

Figure S1. (a) TEM image of oil phase CdSe QDs, Inset: the inter-planer spacing. (b) Diameter of oil phase CdSe QDs.

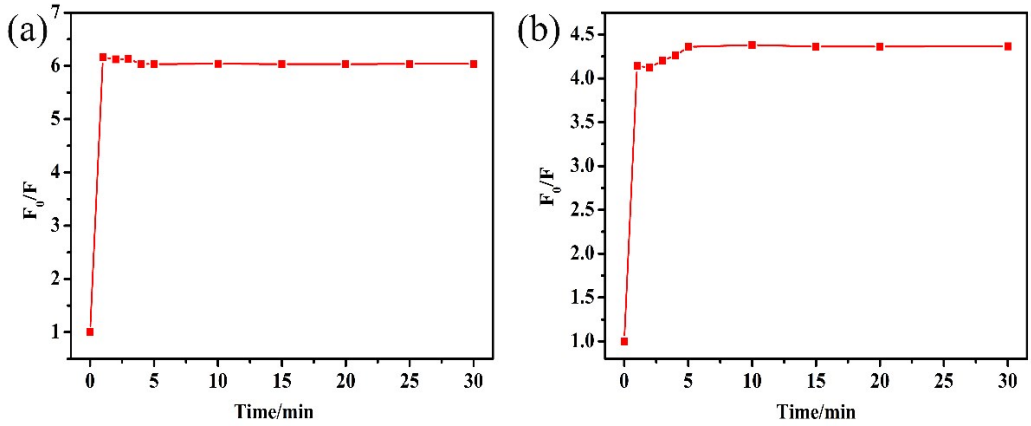

Figure S2. Response time of polymer-capped CdSe/ZnS QDs to Cu^{2+} (a) and Hg^{2+} (b)

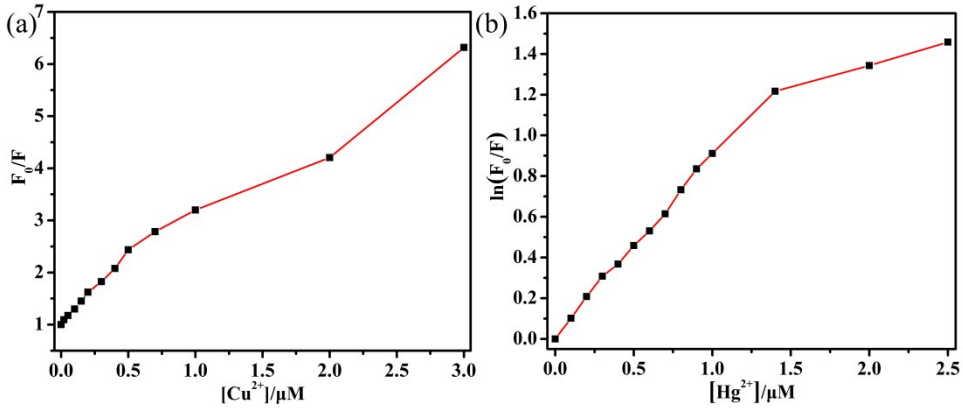

Figure S3. (a) The plot of F/F_0 against the concentration of Cu^{2+}. (b) The plot of ln (F/F_0) against the concentration of Hg^{2+}.

Table S1

Effect of polymer-capped CdSe/ZnS QDs concentration on the detection of Cu^{2+}

[QDs]/10^{-8}M	Detection range	Linear relation(F_0/F)	R^2	LOD (nM)
10	0-0.9 μM	y=1.3x + 0.9388	0.9852	13.62
9	0-0.9 μM	y=1.9x + 0.9160	0.9912	9.32
8	0-0.7 μM	y=2.6x + 1.0499	0.9931	6.81
7	0-0.5 μM	y=4.2x + 0.7543	0.9891	4.21

Table S2

Effect of polymer-capped CdSe/ZnS QDs concentration on the detection of Hg^{2+}

[QDs]/10^{-8}M	Detection range	Linear relation(ln(F_0/F))	R^2	LOD (nM)
6	0-1.5 μM	y=0.46x - 0.0163	0.9979	37.82
5	0-1.4 μM	y=0.63x - 0.0002	0.9973	27.96
4	0-1.4 μM	y=0.87x - 0.0127	0.9971	20.27
3	0-1.0 μM	y=0.99x - 0.0091	0.9952	17.75

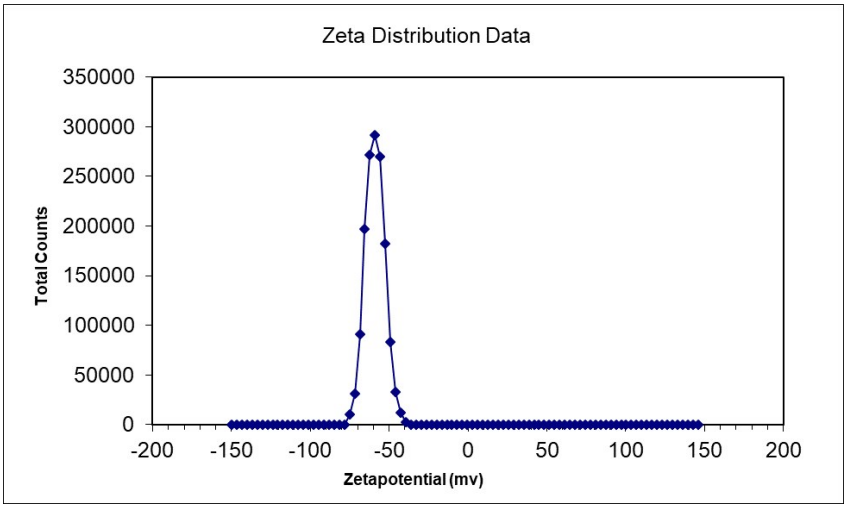

Figure S4. The zeta potential of polymer-capped CdSe/ZnS QDs.

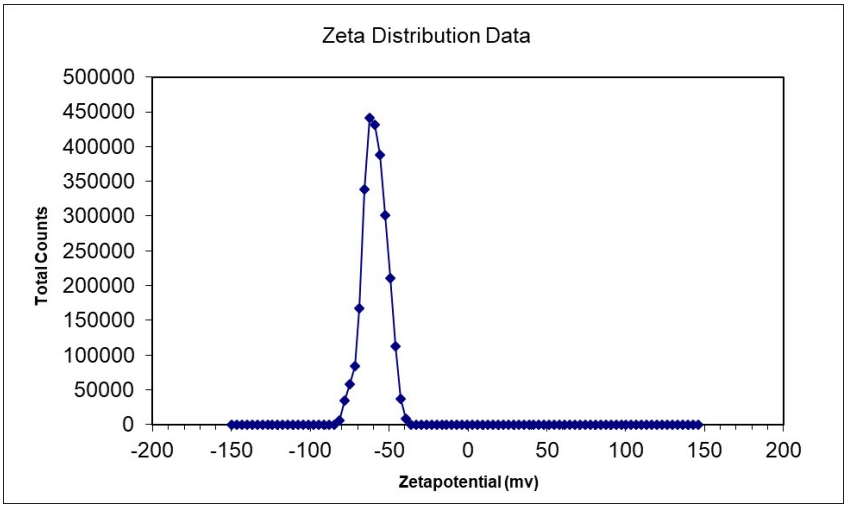

Figure S5. The zeta potential of polymer-capped CdSe/ZnS QDs in the presence of Cu^{2+}.

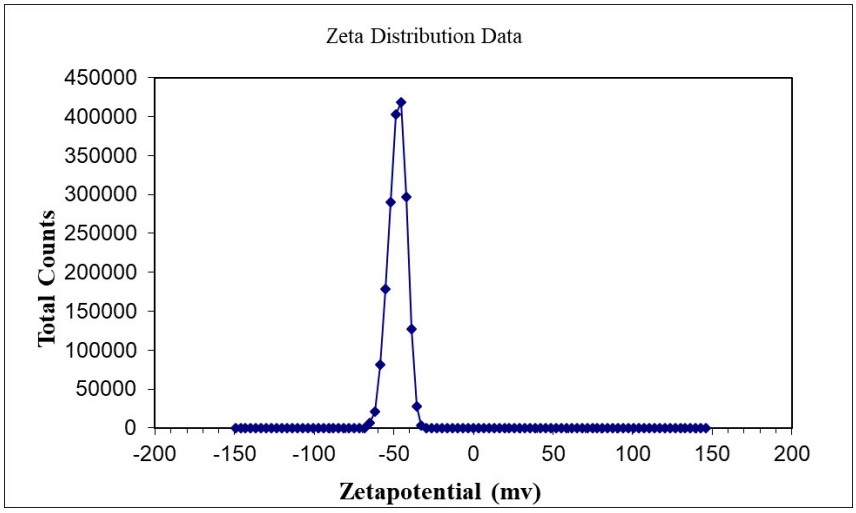

Figure S6. The zeta potential of polymer-capped CdSe/ZnS QDs in the presence of Hg^{2+}.

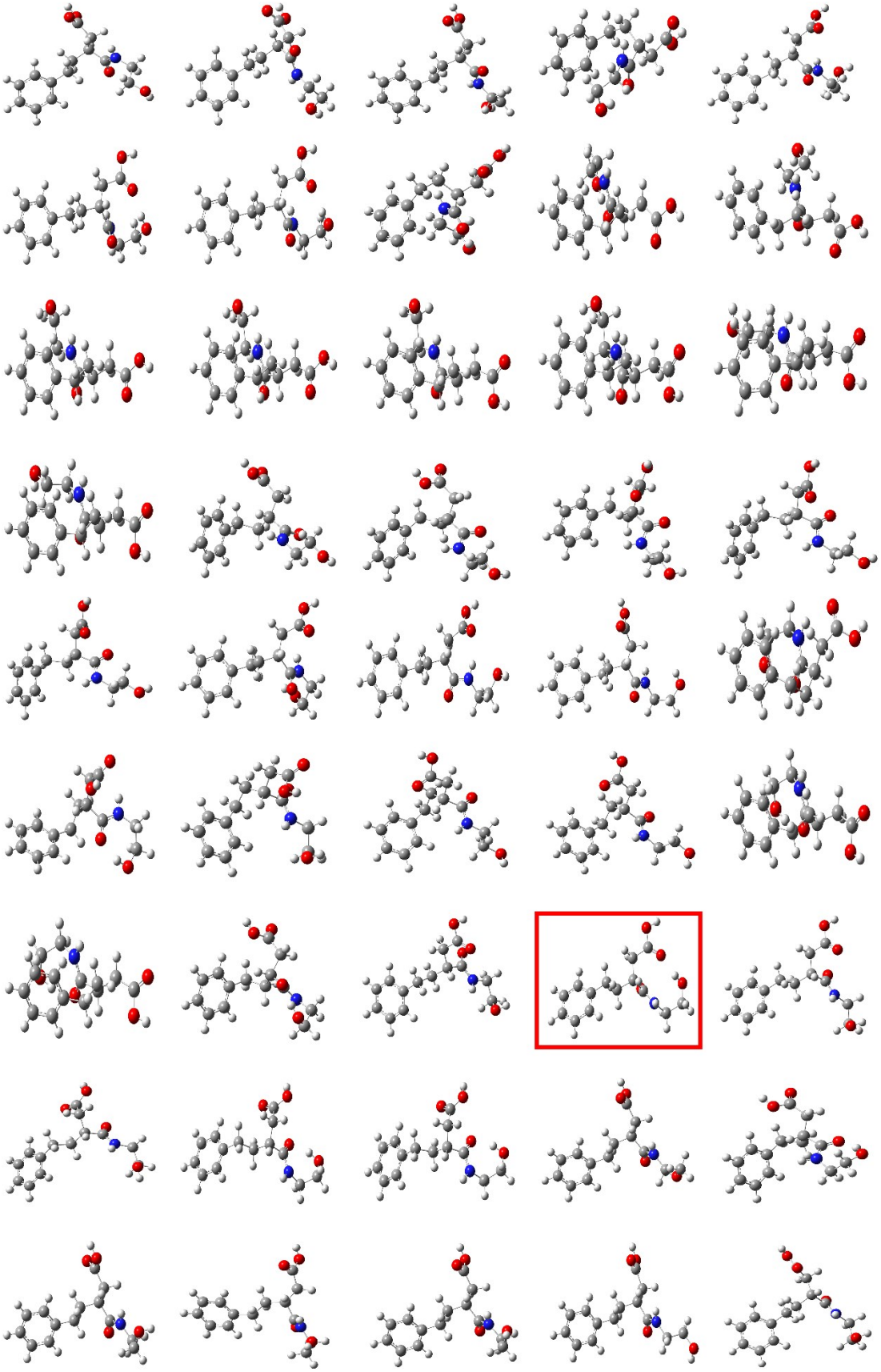

Figure S7. Different optimized structures of the polymer.

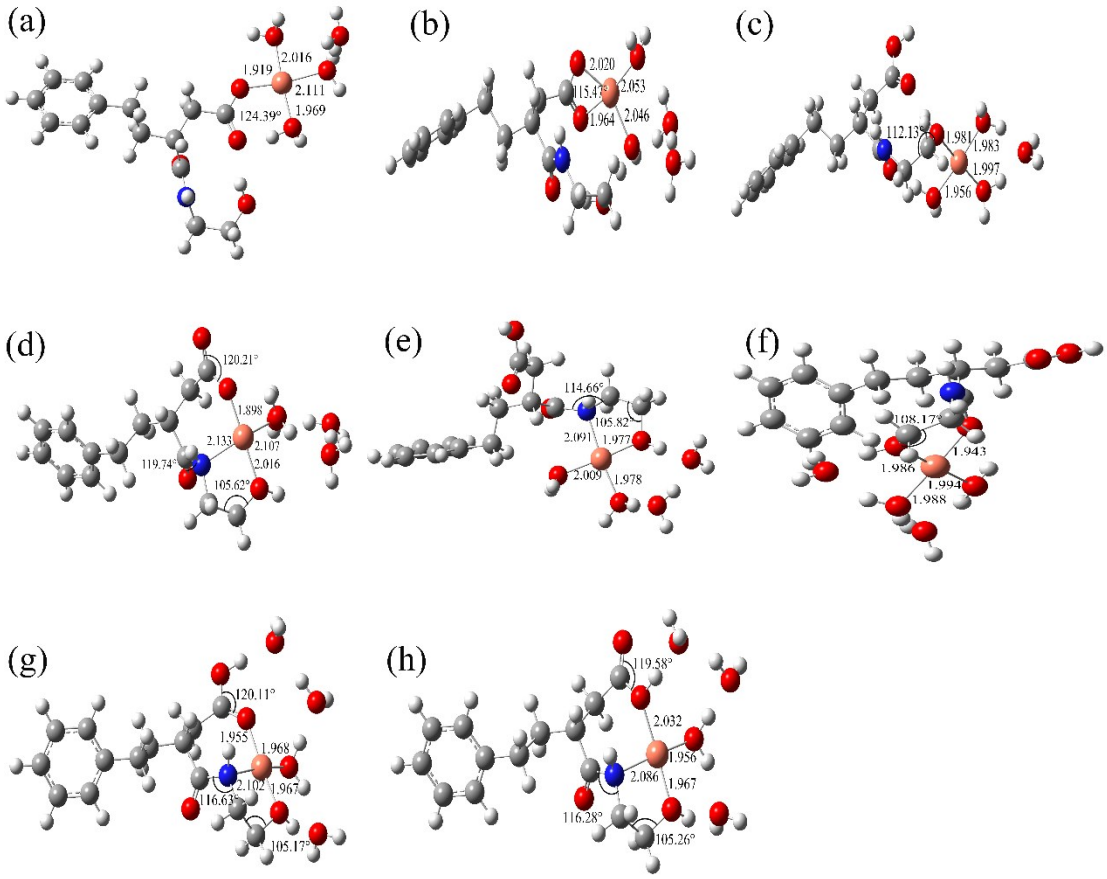

Fig. S8. Different optimized structures of Cu^{2+}- Polymer

Table S3 Coordination energy of polymer with Copper

structure	Δ G (kJ/mol)
a	94.59
b	32.67
c	-58.52
d	47.73
e	5.01
f	-64.31
g	-36.48
h	-3.05

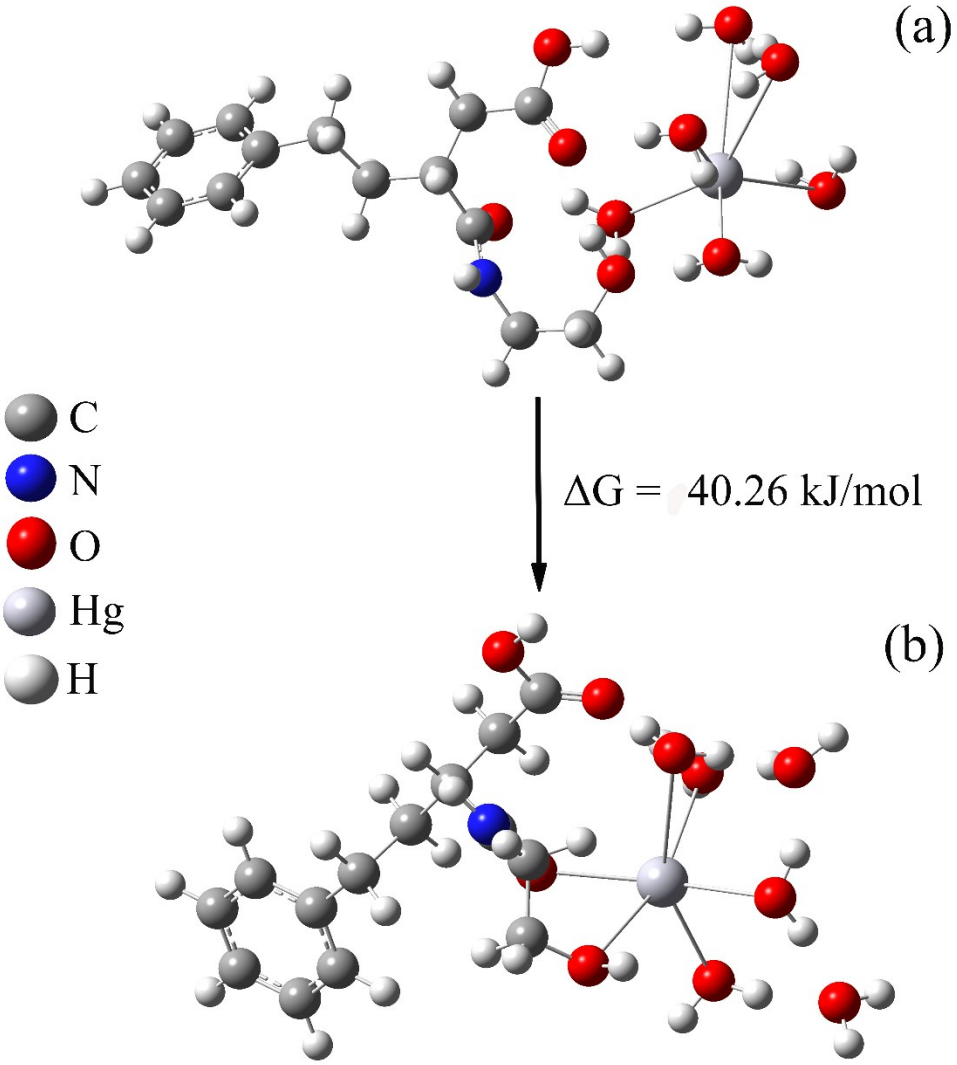

Fig. S9. The optimized structures of (a) Polymer and Hg^{2+}, (b) Hg^{2+}- Polymer.