Supporting Information

4-Mercaptopyridine-Modified Sensor for the Sensitive Electrochemical Detection of Mercury Ions

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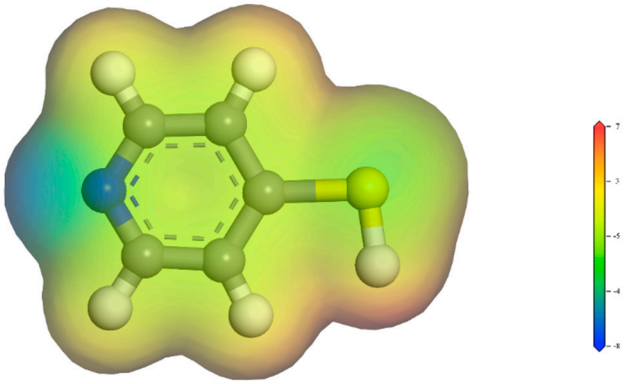


Figure S1. The electrostatic potential diagram of 4-MPY.

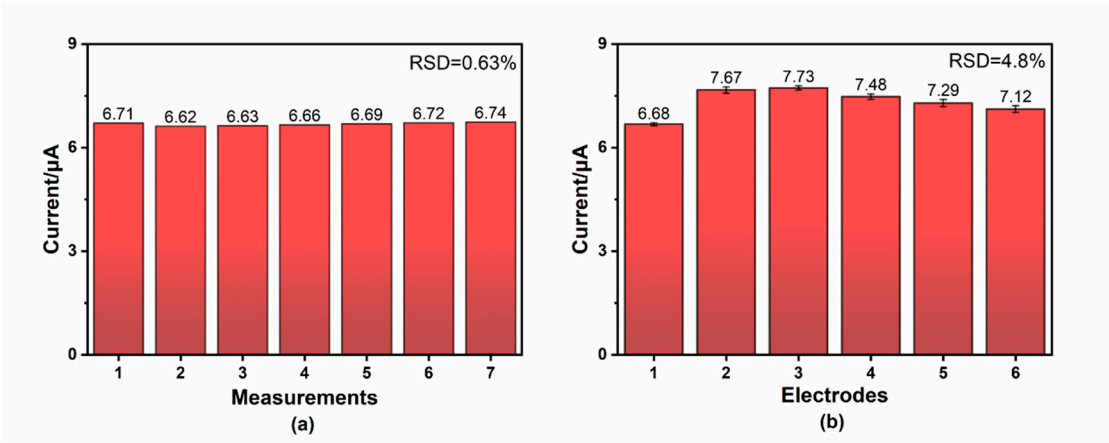


Figure S2. Repeatability and reproducibility study of the proposed sensor. (a) Current intensity in the repeatability experiment of 4-MPY/Au electrode for seven measurements (in 5 mM $[Fe(CN)_6]^{3-/4-}$ with 10 μg/L Hg^{2+}); (b) current intensity in the reproducibility experiment (in 5 mM $[Fe(CN)_6]^{3-/4-}$ with 10 μg/L Hg^{2+}).

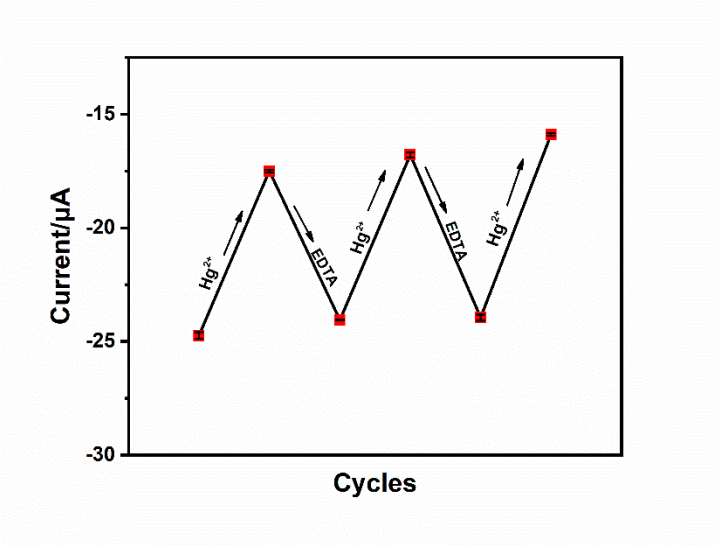


Figure S3. The change of the current intensity in the reusability experiment of 4-MPY/Au electrode with EDTA after reaction with 10 μg/L Hg2+.

Table S1. The impedance fitting parameters of Au electrode surface at different modification conditions.

	R_s /Ω	R_{ct} /Ω
Bare Au	212.5	125.8
4-MPY/Au	204.3	685.7
4-MPY/Au+Hg^{2+}	213.6	812.6

Table S2. Binding energy values of different interferents after reaction with 4-MPY.

Interferents	Complex	E_{M-Py} (Ha)	E_M (Ha)	E_{Py} (Ha)	BE (Ha[1])	BE (kcal/mol)
Hg^{2+}	MPY-Hg^{2+}-MPY	-1942.08	-1714.41	-227.139	-0.53002	-332.591
K^{+}	MPY-K^{+}	-1457.02	-857.211	-599.767	-0.04054	-25.441
Mg^{2+}	MPY-Mg^{2+}-MPY	-1914.07	-1714.41	-199.245	-0.4129	-259.101
Ca^{2+}	MPY-Ca^{2+}-MPY	-2391.61	-1714.41	-676.92	-0.28015	-175.798
Cu^{2+}	MPY-Cu^{2+}-MPY	-1936.5	-1714.41	-221.435	-0.64712	-406.074
Pb^{2+}	MPY-Pb^{2+}-MPY	-1834.57	-1714.41	-119.832	-0.32241	-202.314
Zn^{2+}	MPY-Zn^{2+}-MPY	-1968.4	-1714.41	-253.44	-0.55019	-345.25
Sn^{2+}	MPY-Sn^{2+}-MPY	-1836.45	-1714.41	-121.687	-0.35053	-219.96

[1] 1 Ha = 627.51kcal/mol

Table S3. Stability constants of M^{2+}-pyridine complexes.

M^{2+}	$logK_1$	$logK_2$	Ref
Hg^{2+}	5.1	4.9	1
Zn^{2+}	1.06	0.79	2
Cu^{2+}	2.56	1.89	3

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