Supporting Information

A high-fidelity electrochemical platform based on Au-Se interface for biological detection

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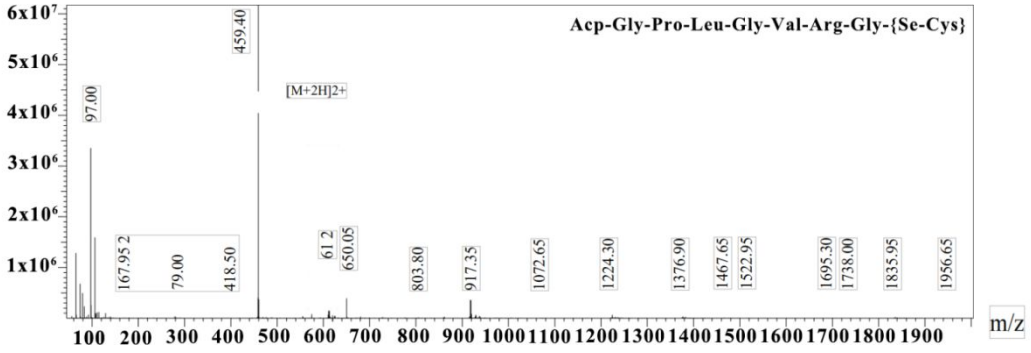

Figure S1. HPLC of the P1: Acp-Gly-Pro-Leu-Gly-Val-Arg-Gly-{Se-Cys}.

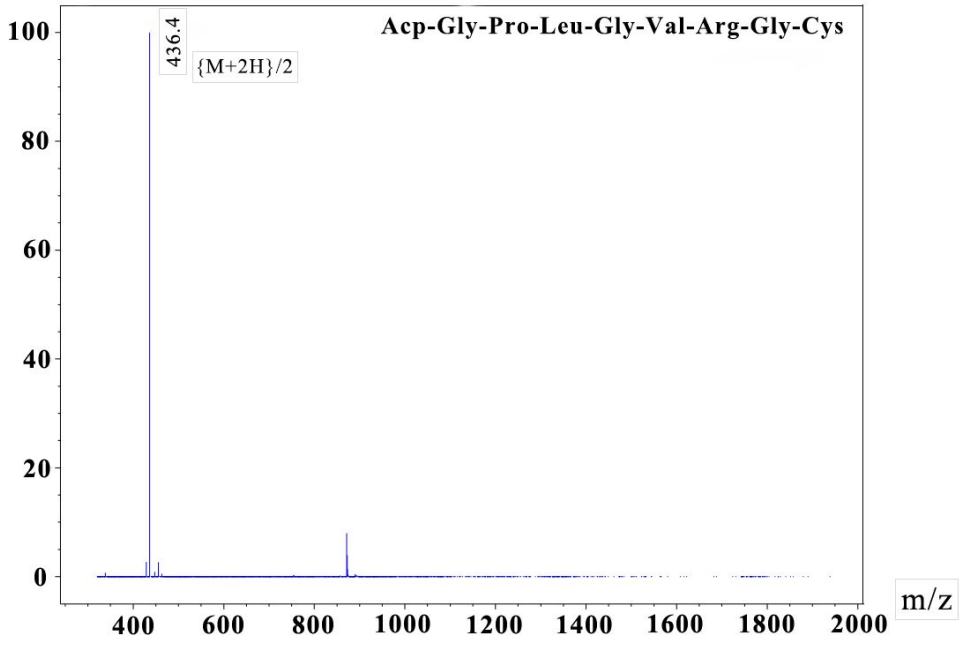

Figure S2. HPLC of the P2: Acp-Gly-Pro-Leu-Gly-Val-Arg-Gly-Cys.

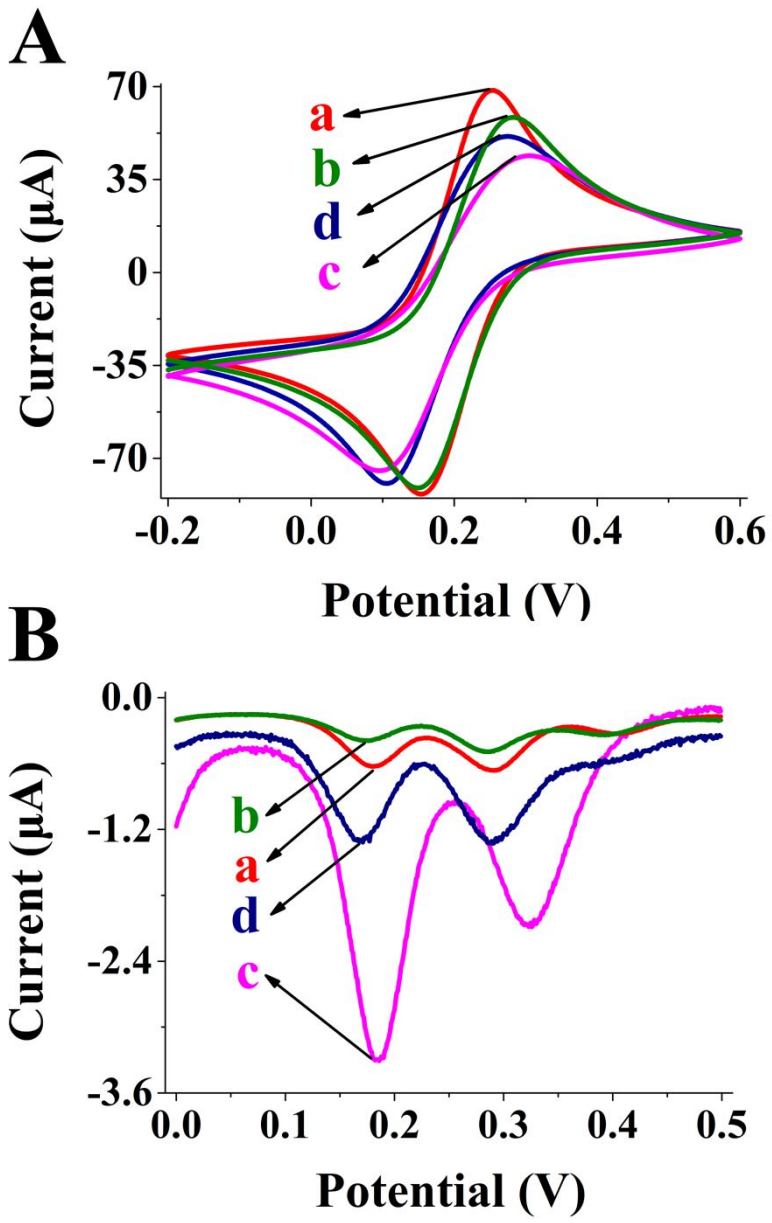

Figure S3. Tracking the assembly of Au-S electrochemical detection platform: (A) CVs of bare Au electrode (a), P2 modified Au electrode (b), ssDNA-P2 modified Au electrode (c) and ssDNA-P2 modified Au electrode incubated with 3.0 nmol/L MMP-2 (d), in 5.0 mmol/L $[Fe(CN)_6]^{3-/4-}$ solution. (B) SWV of bare Au electrode (a), P2 modified Au electrode (b), ssDNA-P2 modified Au electrode (c) and ssDNA-P2

modified Au electrode incubated with 3.0 nmol/L MMP-2 (d), in 0.5 mol/L H_2SO_4 solution containing 5.0 mmol/L $Na_2Mo_2O_3$.

Table S1. Bonding energy and Fermi energy of Au (111) when Au-Se bonds or Au-S bonds are formed with different selenols and thiols compounds. The results are calculated by density functional theory (DFT) with DMol3.

Molecule	**E_B**	**E_F**	**$\Delta E_B = E_B$(Au-Se) – E_B(Au-S)**	**$\Delta E_F = E_F(Au_{-Se}) – E_F(Au_{-S})$**
Au-Se-Hydrogen	0.5470 Ha	-0.1811 Ha	0.0155 Ha	0.0029 Ha
Au-S-Hydrogen	0.5316 Ha	-0.1840 Ha		
Au-Se-Alkane	0.5852 Ha	-0.1795 Ha	0.0159 Ha	0.0023 Ha
Au-S-Alkane	0.5693 Ha	-0.1818 Ha		
Au-Se-Aromatics	0.5185 Ha	-0.1207 Ha	0.0384 Ha	0.0023 Ha
Au-S-Aromatics	0.4800 Ha	-0.1230 Ha		
Au-Se-Peptide	0.5697 Ha	-0.1728 Ha	0.0433 Ha	0.0025 Ha
Au-S-Peptide	0.5264 Ha	-0.1753 Ha		

E_B, the bonding energy of Au (111) with different selenols and thiols compounds. E_F, the Fermi energy of Au (111) connected with different selenols and thiols compounds. E_B (Au-Se), the bonding energy of Au (111) with different selenols compounds. E_B (Au-S), the bonding energy of Au (111) with different thiols compounds. E_F (Au_{-Se}), the Fermi energy of Au (111) connected with different selenols compounds. E_F (Au_{-S}), the Fermi energy of Au (111) connected with different thiols compounds.

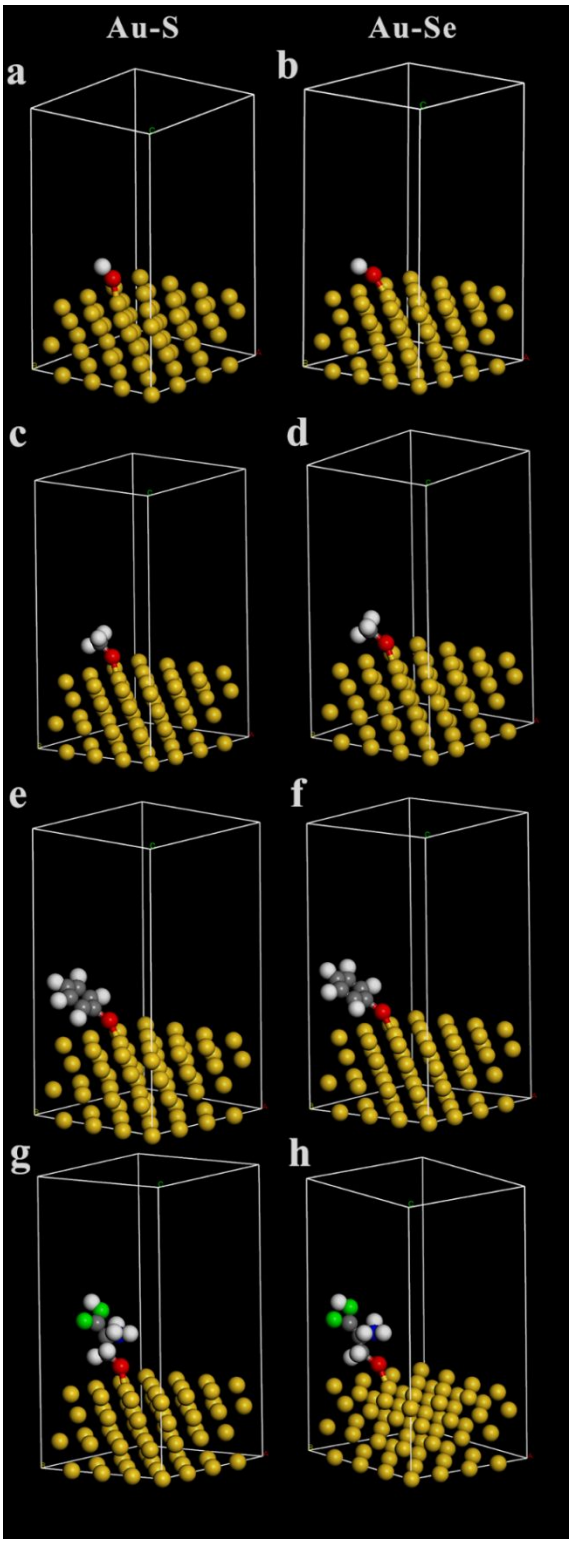

Figure S4. The spatial structures of sulfhydryl group (a), selenyl group (b), alkanethiolate (c), alkaneselenolate (d), benzenethiol (e), benzeneselenol (f), Cys (g), Se-Cys (h) on the Au (111) surface. The results are calculated by density functional theory (DFT) with DMol3.