Efficient Chemodosimeter for Hg(II) Via Diselenide Oxidation

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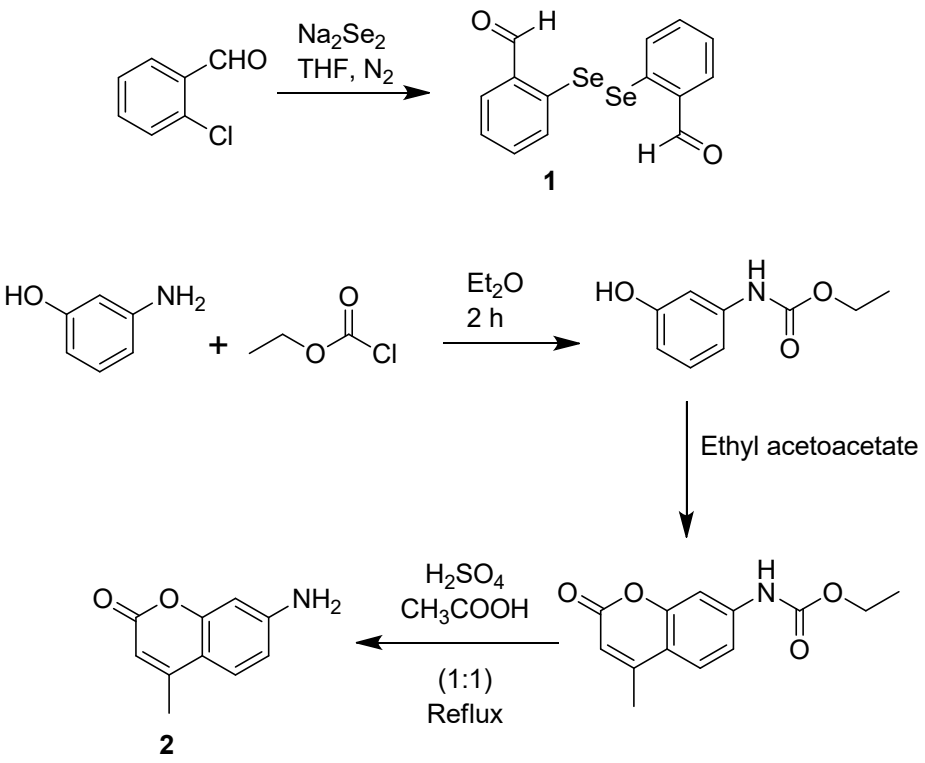

Scheme S1. Synthesis of compounds **1** and **2**.

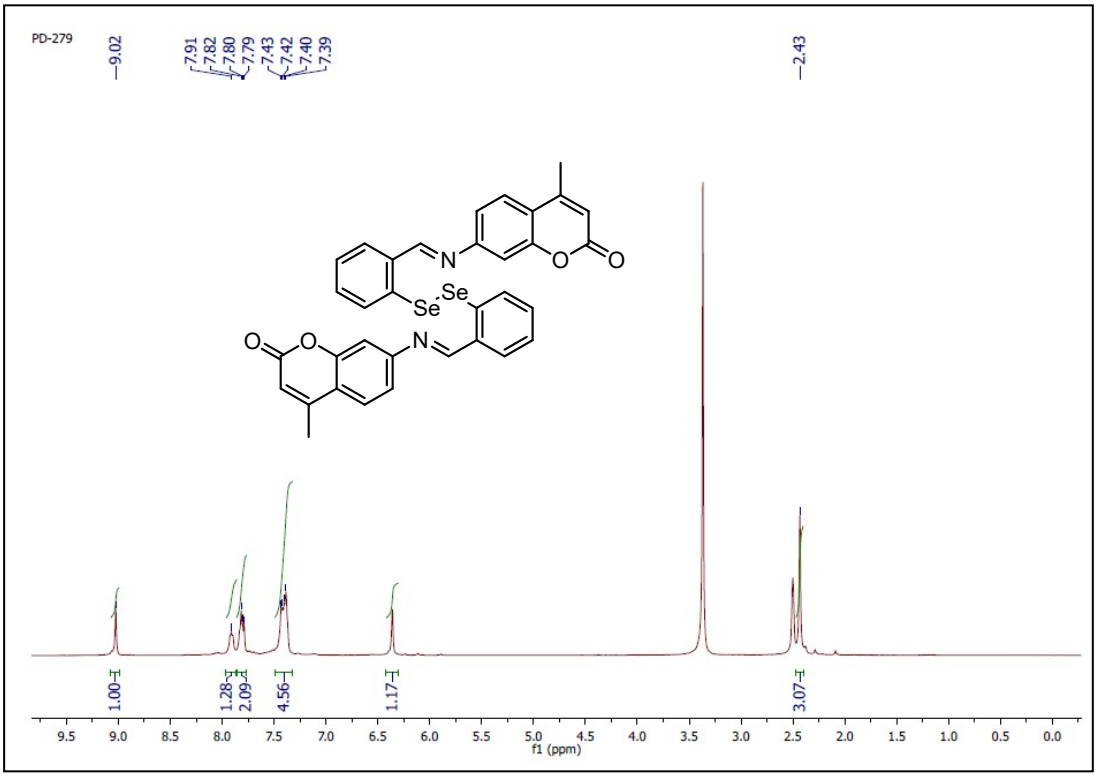

Fig. S1. ^{1}H NMR spectrum of probe **3**.

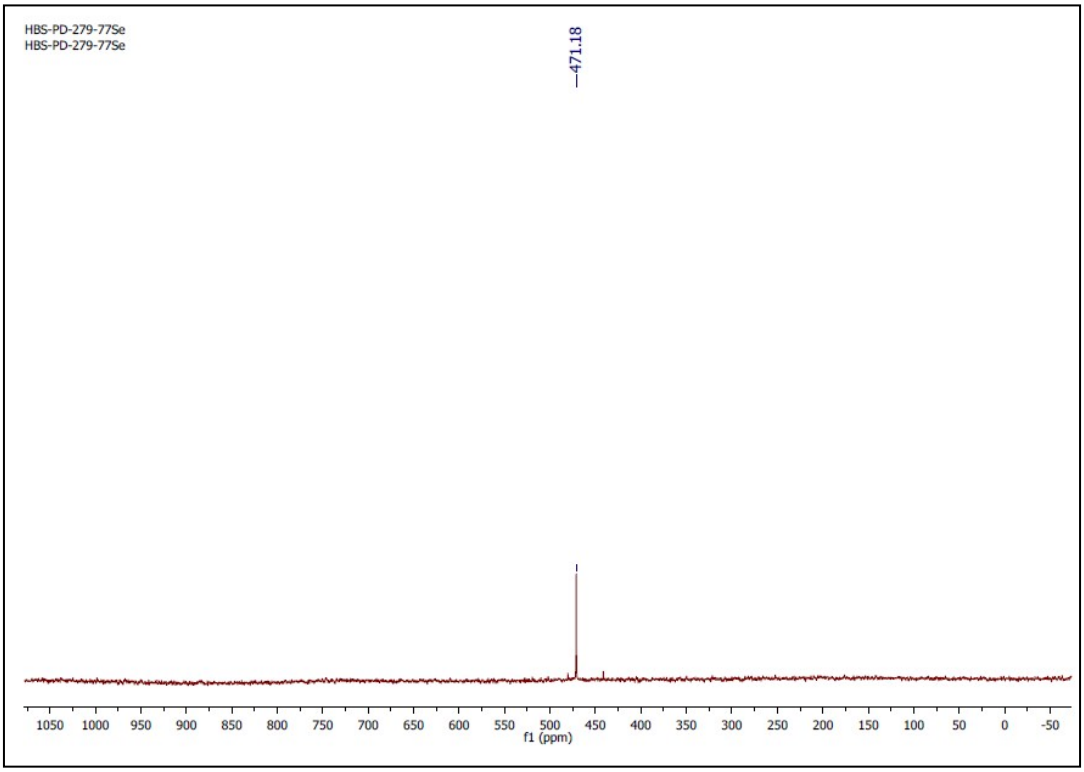

Fig. S2. ^{77}Se NMR spectrum of probe **3**.

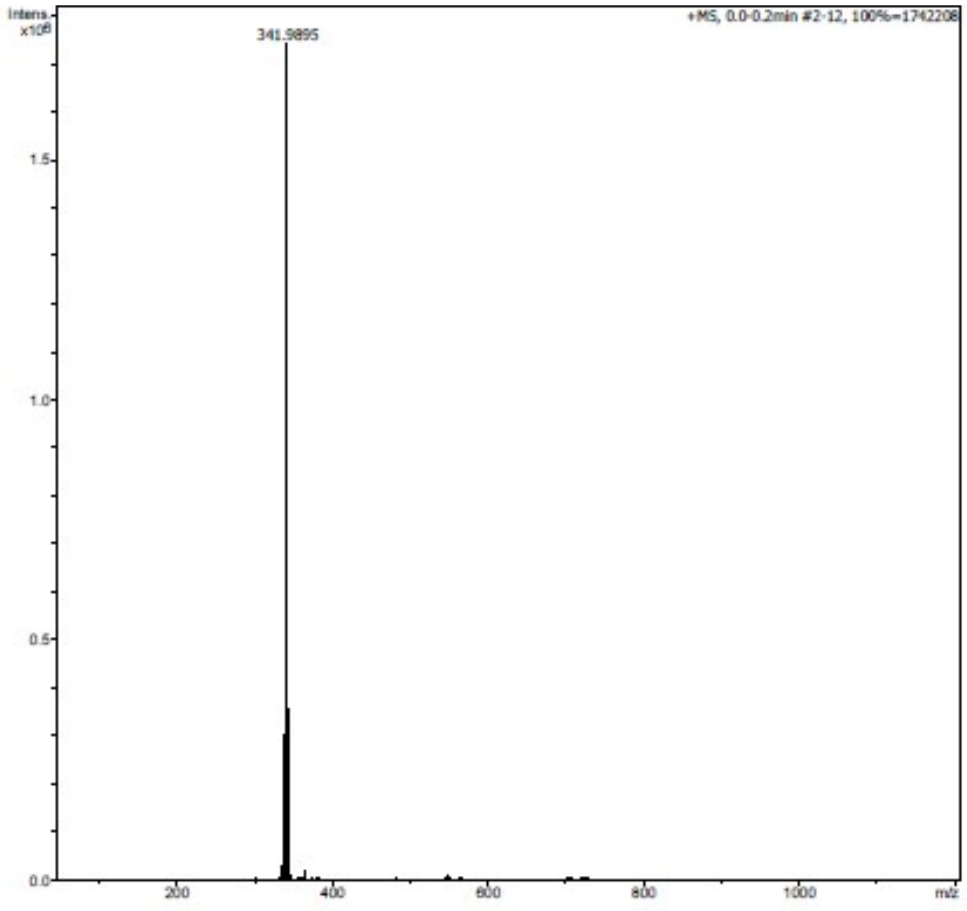

Fig. S3. Mass spectrum of probe **3**.

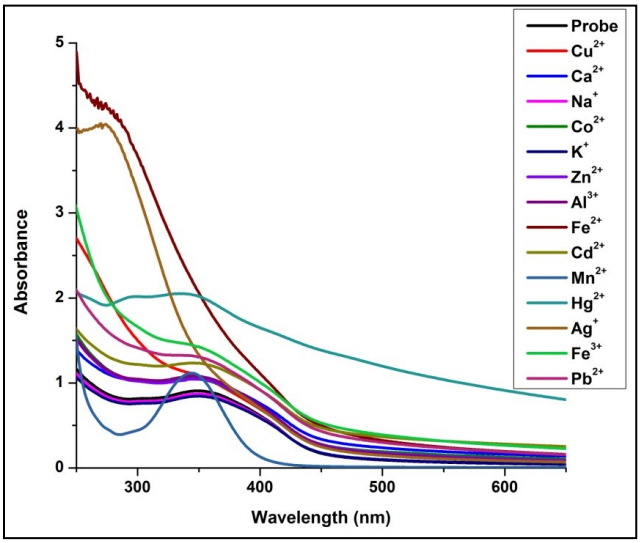

Fig. S4. UV-vis spectral changes of probe (30 μM) in PBS pH=7.4 with metal ions at rt incubated for 20 min at room temperature; slit width Ex./Em.= 2.5/2.5 nm.

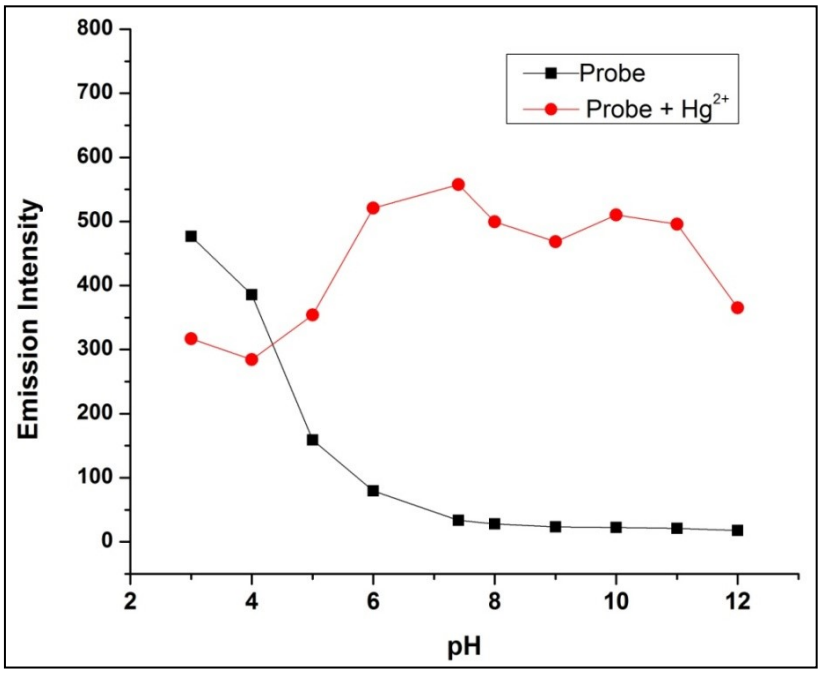

Fig. S5. Plot of emission intensity Vs pH for probe **3**.

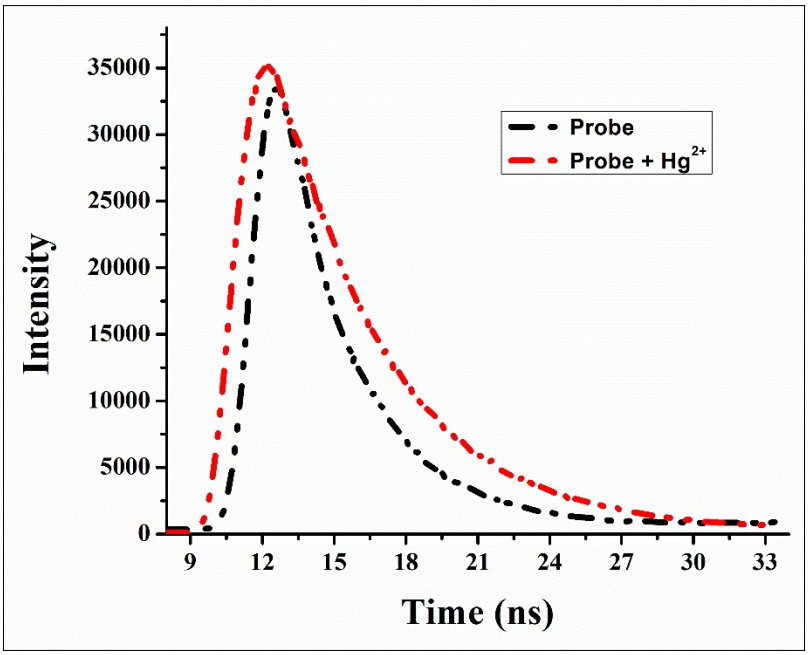

Fig. S6. Fluorescence lifetime measurement of probe and probe with Hg^{2+}.

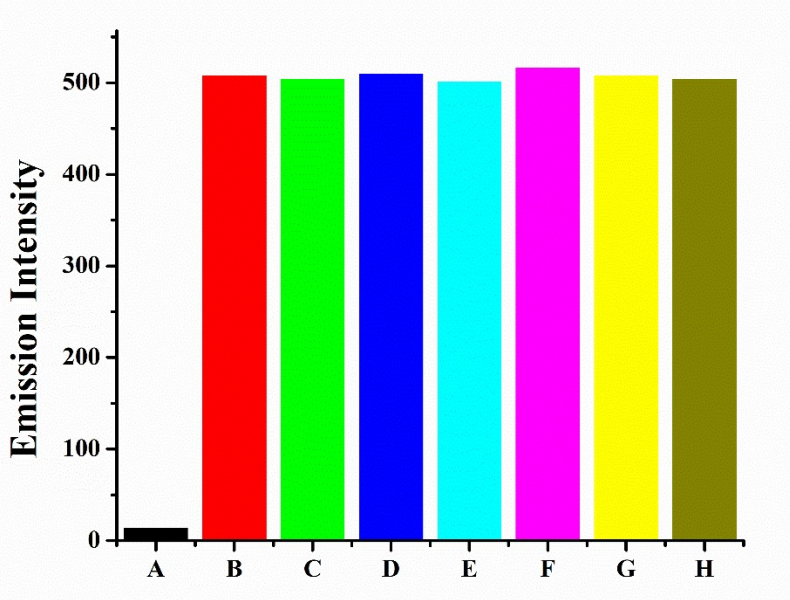

Fig. S7. Fluorescence spectra after addition of biothiols (DL-homocysteine, L-cysteine, GSH, N-acetyl- L-cysteine, D-methionine and Na_2S) to the probe **3** (30 μM) and Hg^{2+}, incubated for 30 min at rt (λ_{ex} = 348 nm, λ_{em}= 438 nm), slit width 2.5/2.5 nm (A = Probe **3**, B = Probe **3** + Hg^{2+}, C = Probe **3** + Hg^{2+} + DL-homocysteine, D= Probe **3** + Hg^{2+} + L-cysteine, E = Probe **3** + Hg^{2+} + GSH, F = Probe **3** + Hg^{2+} + N-acetyl-L-cysteine, G = Probe **3** + Hg^{2+} + Dmethionine, H = Probe **3** + Hg^{2+} + Na_2S).

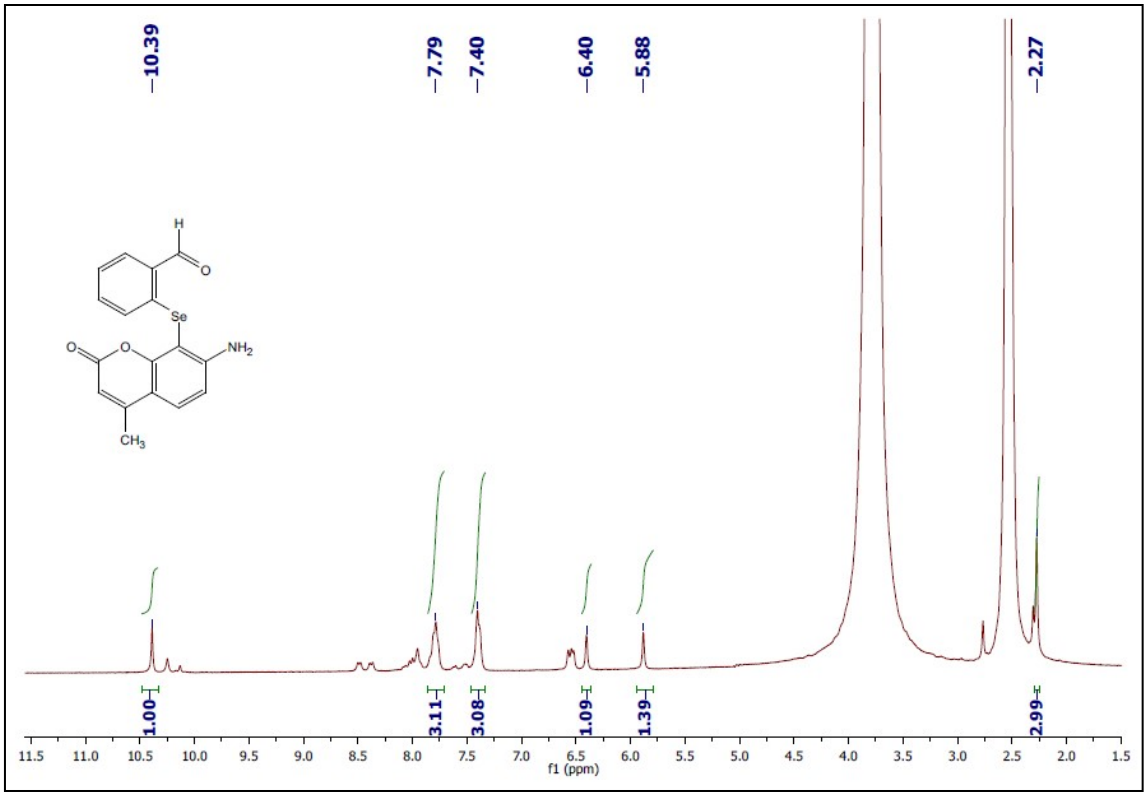

Fig. S8. ^{1}H NMR spectrum of compound **4**.

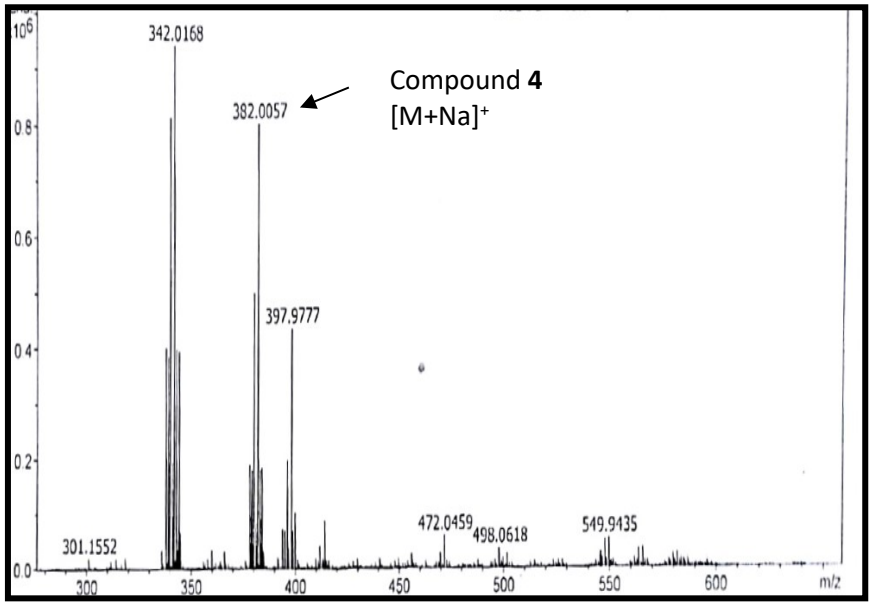

Fig. S9. Mass spectrum of compound **4**.

Table S1. Crystal data and structural refinements for compound **4**.

Formula	$C_{17}H_{14}NO_3Se$	*V[Å³]*	1466.92(18)
Mr	345.01	*Z*	4
system	Monoclinic	Size [mm³]	0.170 x 0.106 x 0.036
space group	P–1	*ρ*calcd [Mg/m³]	1.627
a [Å]	7.7511(5)	*μ [mm–1]*	2.572
b [Å]	23.9217(13)	Refls. collected	31198
c [Å]	8.4244(6)	Independent reflections	3776 [R(int) = 0.1384]
α [°]	90	*R1 [I>2σ(I)]*	0.0677
β [°]	110.099	*wR2 [I>2σ(I)]*	0.1495
γ [°]	90		