Supplementary Material (ESI) for New Journal of Chemistry

Supporting information

A new squaraine and Hg^{2+}-based chemosensor with tunable measuring range for thiol-containing amino acids

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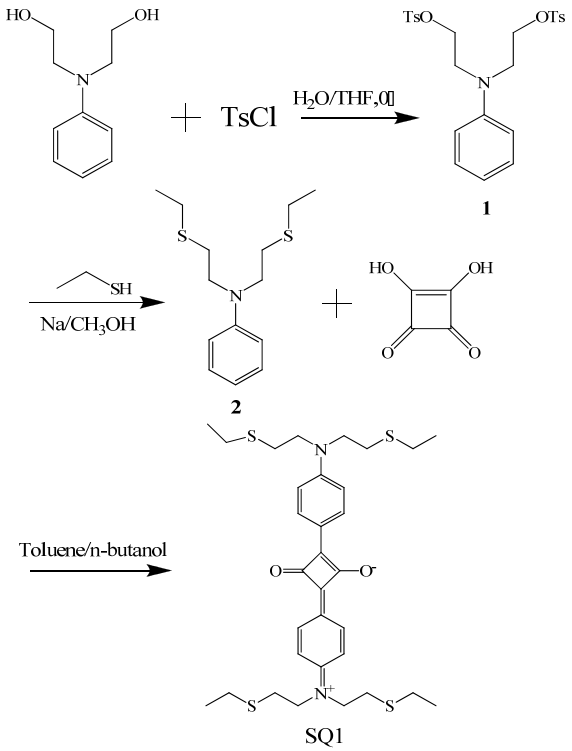
Synthesis of SQ1

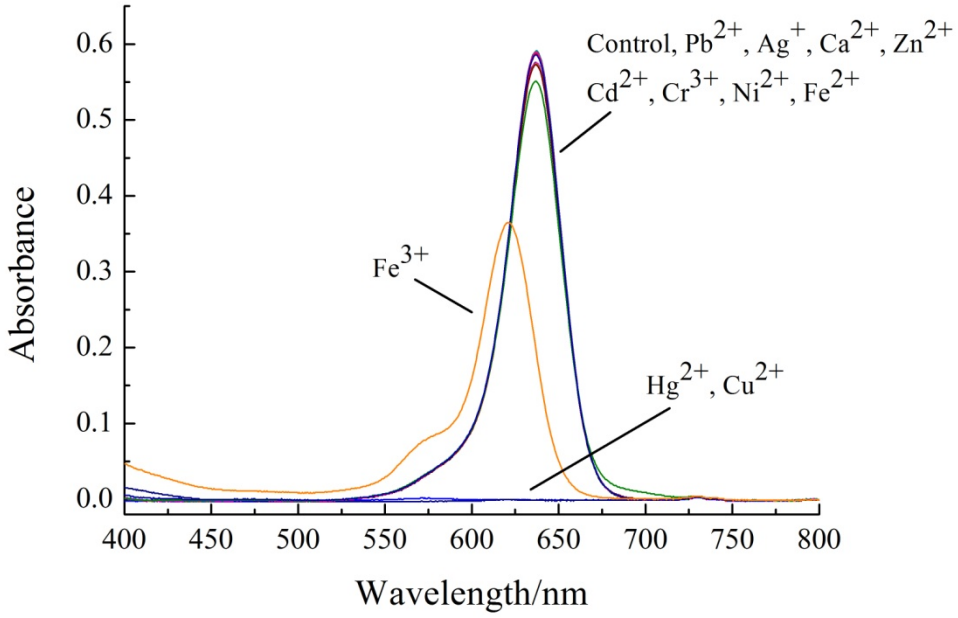
Scheme S1 shows the method that we used to synthesize SQ1. Compounds **1** and **2** were synthesized according to the reported literatures.[1] SQ1 was then obtained by the condensation of **2** with squaric acid in *n*-butanol/toluene (1:1 v/v) under reflux. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.47 (d, 4H, J = 8.7 Hz), 6.89 (d, 4H, J = 9.08 Hz), 3.73 (t, 8H, J = 7.28 Hz), 2.80 (t, 8H, J = 7.64 Hz), 2.62 (q, 8H, J = 7.40 Hz), 1.30 (t, 12H, J = 7.36 Hz). MS (ESI): calcd for ($C_{32}H_{44}N_2O_2S_4$+ H^+) 617.2364, found 617.2380.



Scheme S1. Synthetic route of SQ1.

Spectroscopic response of SQ1 in acetonitrile toward metal ions

(a)



(b)

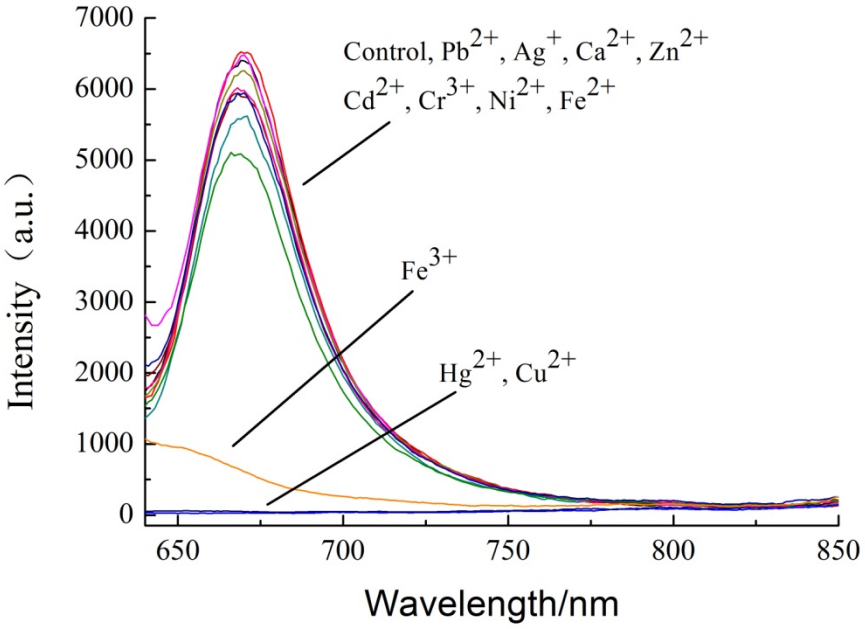


Figure S1. Absorption (a) and fluorescence (b) spectra of SQ1(2 μM) in acetonitrile upon addition of various metal ions (40 μM).

Spectroscopic response of SQ1 in acetonitrile/water (2:1) toward metal ions

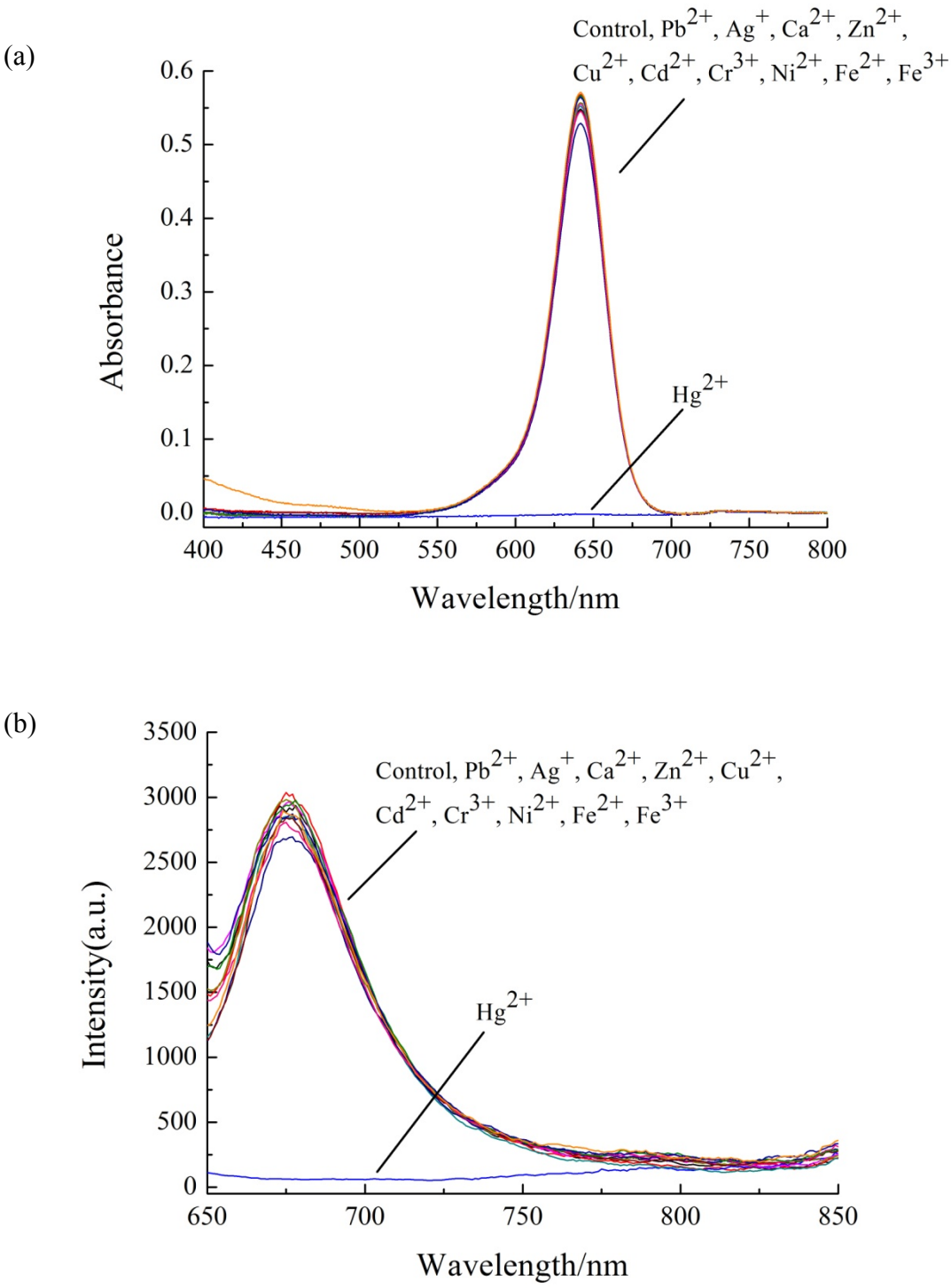


Figure S2. Absorption (a) and fluorescence (b) spectra of SQ1(2 μM) in acetonitrile/water (2:1 in volume ratio) upon addition of various metal ions (40 μM).

Spectroscopic response of SQ1 in acetone toward metal ions

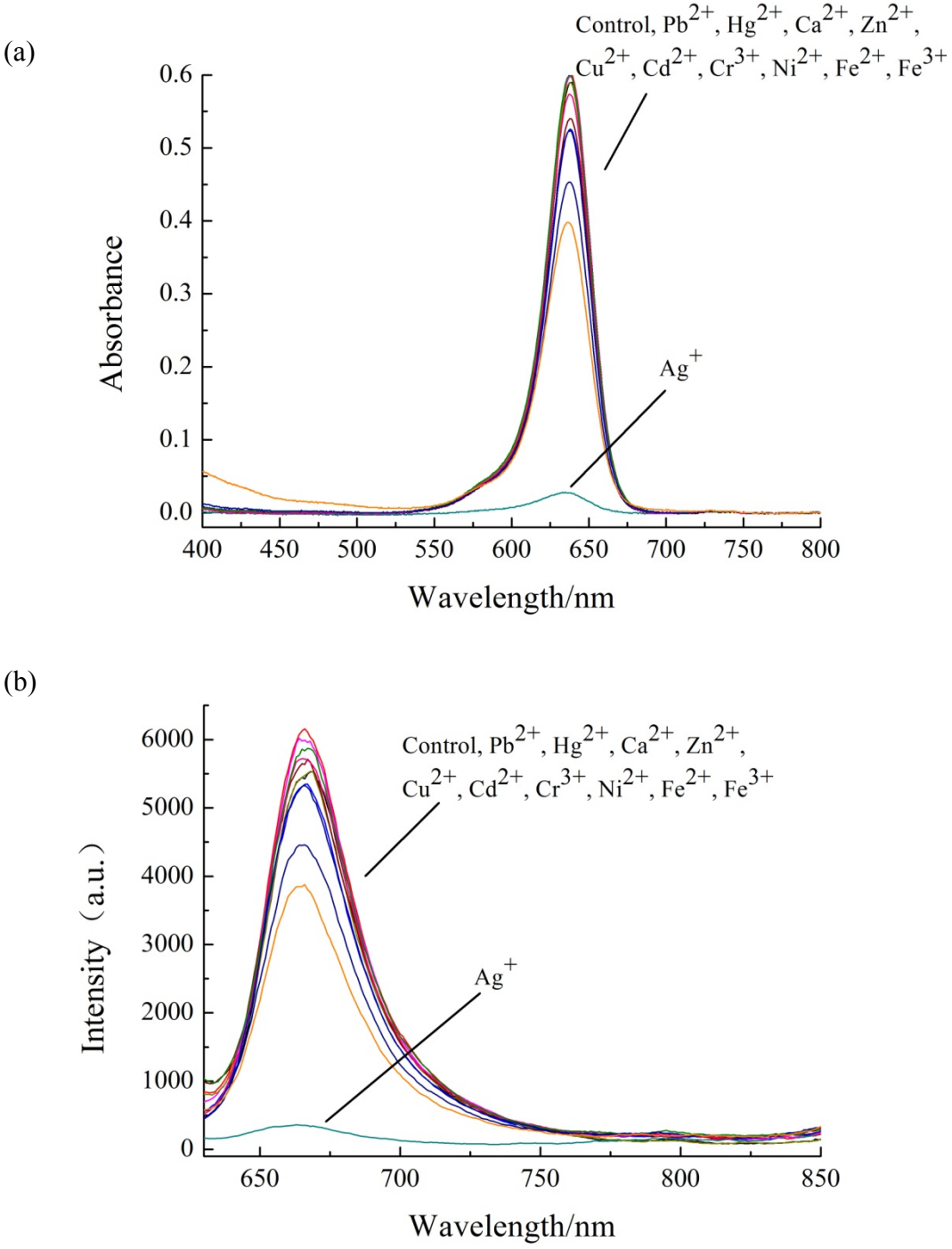


Figure S3. Absorption (A) and fluorescence (B) spectra of SQ1(2 μM) in acetone upon addition of various metal ions (40 μM).

Spectroscopic response of SQ1 and Hg^{2+} solution in acetonitrile/water toward cysteine

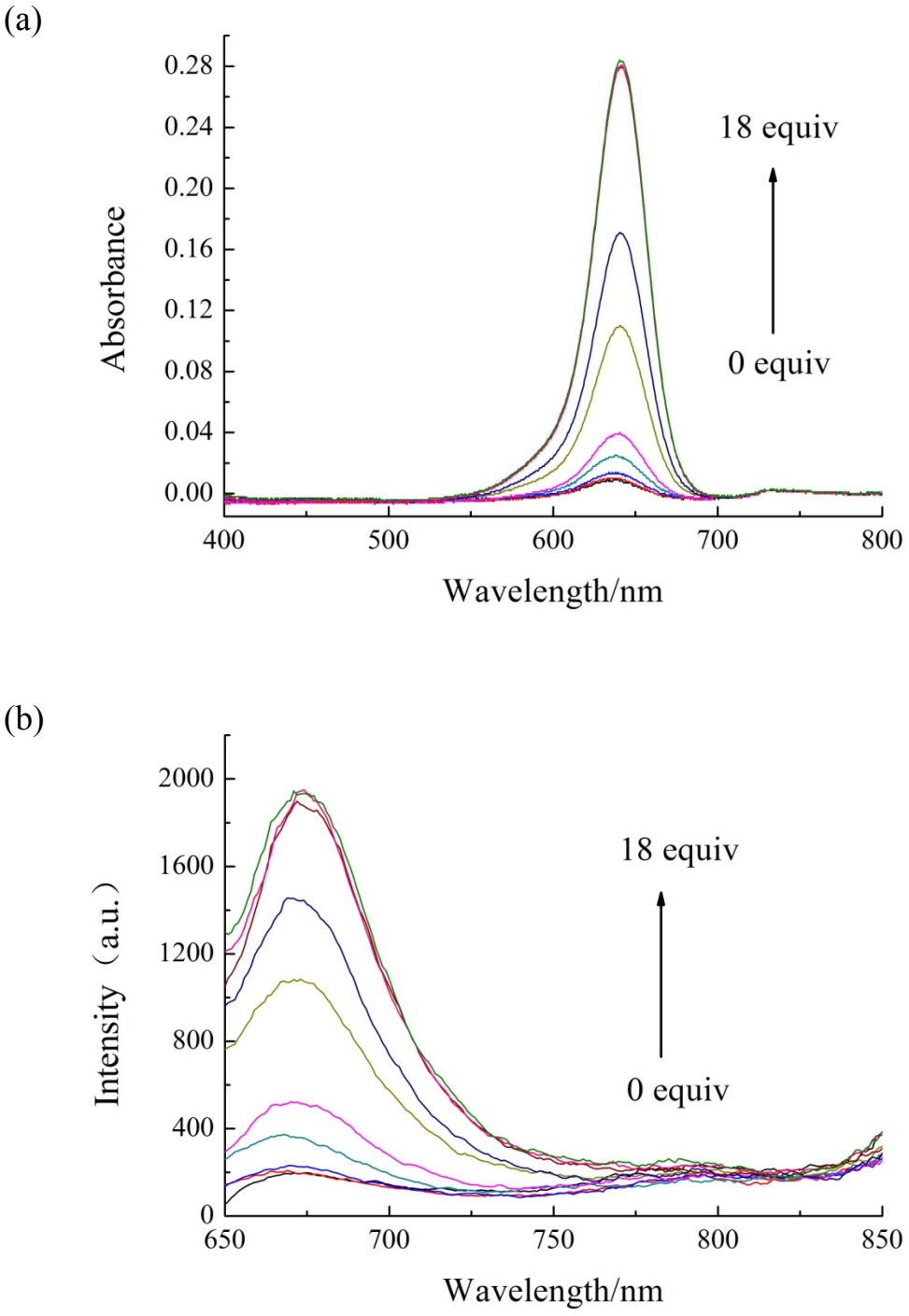


Figure S4. Absorption (a) and emission (b) recovery of the solution of SQ1 (1 μM) and Hg^{2+} (20 μM) in acetonitrile/water (2:1) upon addition of cysteine.

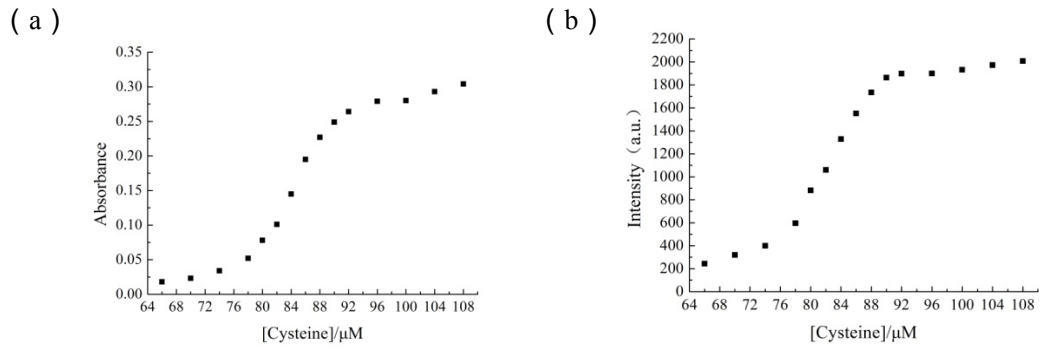


Figure S5. Absorbance at 642 nm (a) and fluorescence intensity at 678 nm of the acetonitrile/water solutions (2:1) of SQ1 (1 μM) and Hg^{2+} (120 μM) in the presence of varied concentrations of cysteine.

Reference

1. J. Ishikawa, H. Sakamoto, T. Mizuno, M. Otomo, *Bull. Chem. Soc. Jpn.*, 1995, **68**, 3071.