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Supporting Information

Dual functions of metal ion detection and antibacterial activity of sulfur quantum dots

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Experimental

Determination of cytotoxicity by MTT assay

L929 fibroblasts were used to evaluate the biocompatibility of the SQDs. For this, L929 cells were cultured in Dulbecco's modified Eagle medium (DMEM) (Corning, Glendale, AZ, USA) supplemented with 10% fetal bovine serum (Gibco, Franklin Lakes, NJ, USA) and 1% antibiotic/antimycotic solution in a humidified incubator with 5% CO₂ at 37 °C. The medium was refreshed every two days until 80% cell confluence was achieved. The 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-tetrazolium bromide (MTT) assay is an indirect cell viability measurement that uses the reaction of mitochondrial dehydrogenase to reduce tetrazolium salts to insoluble formazan (purple compound) in metabolically active cells. For the MTT test, L929 cells (7×10^3 cells/well) were seeded in 96-well plates and incubated overnight. Then the cells were treated with different concentrations of SQDs (up to a maximum concentration of 2000 µg/mL) for 72 hours. After the treatment, 20 µL of 2 mg/mL MTT solution was added to each well and incubated at 37 °C for three hours. After dissolving formazan crystals with DMSO, the absorbance was monitored at 570 nm using a microplate reader (Molecular Devices, CA, USA). Data were presented as mean \pm standard deviation (SD) from at least three independent experiments in triplicate.

Results



Figure S1 (a) Selectivity of SQDs in the presence of various metal ions, (b) Interference evaluation of SQDs+Pb(II) in the presence of interferents (1:3) (c) Interference evaluation of SQDs+Bi(III) in the presence of interferents.

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Figure S2. Stern-Volmer plots of SQDs in the presence of (a) Pb(II) and (b) Bi(III).



Figure S3. pH effect on SQDs emission and sensing to (a) Pb(II) and (b) Bi(III) ions. The test was performed in triplicate (n=3).



Figure S4. Conentration-dependent and normalized TRPL spectral titrations for (a) SQDs and SQDs+Pb(II) and (b) SQDs and SQDs+Bi(III).

| Sample | τ_1 | $	au_2$ | τ_3 | T _{avg} |
|----------------------|----------|---------|----------|------------------|
| SQDs | 0.395 | 1.782 | 7.702 | 4.012 |
| SQDs+Pb (II) 25 μM | 0.360 | 1.909 | 8.068 | 4.431 |
| SQDs+Pb (II) 50 µM | 0.443 | 1.467 | 7.278 | 3.992 |
| SQDs+Pb (II) 75 µM | 0.464 | 1.845 | 8.449 | 4.489 |
| SQDs+Pb (II) 100 μM | 0.446 | 1.854 | 8.411 | 4.621 |
| SQDs+Pb (II) 125 μM | 0.428 | 1.978 | 8.659 | 4.590 |
| SQDs+Pb (II) 150 μM | 0.388 | 1.990 | 8.932 | 4.527 |
| SQDs+Pb (II) 175 μM | 0.369 | 1.962 | 8.311 | 4.500 |
| SQDs+Pb (II) 200 μM | 0.519 | 1.689 | 7.999 | 4.499 |
| SQDs+Pb (II) 225 μM | 0.380 | 2.163 | 9.164 | 4.457 |
| SQDs+Pb (II) 250 μM | 0.311 | 1.788 | 7.38 | 4.247 |
| SQDs+Bi (III) 25 μM | 0.173 | 2.053 | 8.021 | 4.226 |
| SQDs+Bi (III) 50 µM | 0.452 | 1.756 | 7.764 | 4.427 |
| SQDs+Bi (III) 75 μM | 0.286 | 1.888 | 7.736 | 4.164 |
| SQDs+Bi (III) 100 μM | 0.258 | 1.917 | 7.775 | 4.149 |
| SQDs+Bi (III) 125 μM | 0.611 | 1.050 | 5.792 | 3.742 |
| SQDs+Bi (III) 150 μM | 0.326 | 1.808 | 8.144 | 4.352 |
| SQDs+Bi (III) 175 μM | 0.288 | 1.472 | 6.289 | 3.645 |
| SQDs+Bi (III) 200 µM | 0.453 | 1.196 | 5.507 | 3.625 |
| SQDs+Bi (III) 225 μM | 0.304 | 2.001 | 9.213 | 4.297 |
| SQDs+Bi (III) 250 μM | 0.365 | 1.384 | 6.439 | 3.779 |



Figure S5. HR-TEM images of SQDs in the presence of Pb(II) and Bi(III) ions.

Table S1. Fitted decay constants of SQDs with Pb(II) and Bi(III) ions from TRPL data.



Figure S6. Influence of metal ions on the size of SQDs via DLS (a) SQDs (b) SQDs+Pb(II)
(125 μM) (c) SQDs+Bi(III) (125 μM) and zeta potential of SQDs (d) SQDs+Pb(II) (125 μM)
(e) and SQDs+Bi(III) (125 μM) (f).



Figure S7. FTIR spectra of SQDs in the presence and absence of metal ions.

| Sample | PLQY | Sample | PLQY |
|---------------------|-------|----------------------|-------|
| SQDs | 11.42 | SQDs | 11.42 |
| SQDs+Pb(II)(25 µM) | 6.26 | SQDs+Bi(III)(25 µM) | 4.84 |
| SQDs+Pb(II)(50 µM) | 5.78 | SQDs+Bi(III)(50 µM) | 4.01 |
| SQDs+Pb(II)(75 µM) | 3.77 | SQDs+Bi(III)(75 µM) | 3.27 |
| SQDs+Pb(II)(100 µM) | 2.05 | SQDs+Bi(III)(100 µM) | 2.40 |
| SQDs+Pb(II)(125 µM) | 1.39 | SQDs+Bi(III)(125 µM) | 1.86 |
| | | | |

Table S2. Influence of Pb(II) and BI(III) ions on PLQY of SQDs.



Figure S8. Effect of metal ions on QY of SQDs: (a) SQDs+Pb(II) (b)SQDs+Bi(III).



Figure S9. (a) Luminescence response of SQDs for 90 days, the effect of (b) temperature, and (c) NaCl on SQDs emission property. The test was performed in triplicate (n=3).