

## Rhodamine-Modified Upconversion Nanoprobe for Distinguish $\text{Cu}^{2+}$ from $\text{Hg}^{2+}$ and Living Cells Imaging

Yanxia Xu<sup>a</sup>, Huifang Li<sup>b</sup>, Xianfu Meng<sup>a</sup>, Jinliang Liu<sup>\*a</sup>, Lining Sun<sup>a</sup>, Xiaolin Fan<sup>b</sup>  
and Liyi Shi<sup>\*a</sup>

<sup>a</sup> Research Center of Nano Science and Technology, Shanghai University, 200444, China.

<sup>b</sup> Key Laboratory of Organo-Pharmaceutical Chemistry, Gannan Normal University, Ganzhou 341000, P. R. China.

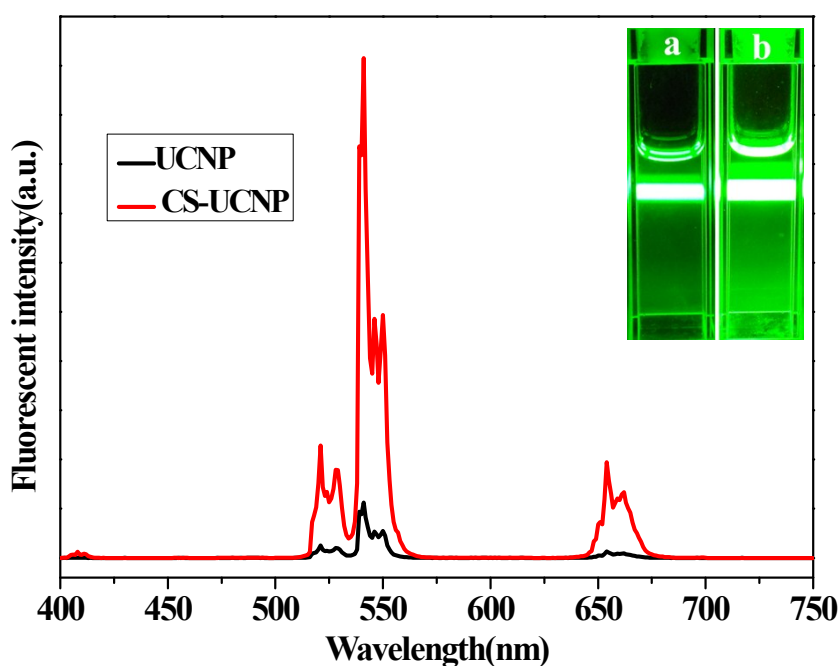


Fig. S1 Upconversion luminescence spectra of UCNP and CS-UCNP. Inset shows the fluorescent pictures of UCNP (a) and CS-UCNP (b) in cyclohexane under 980 nm NIR excitation.

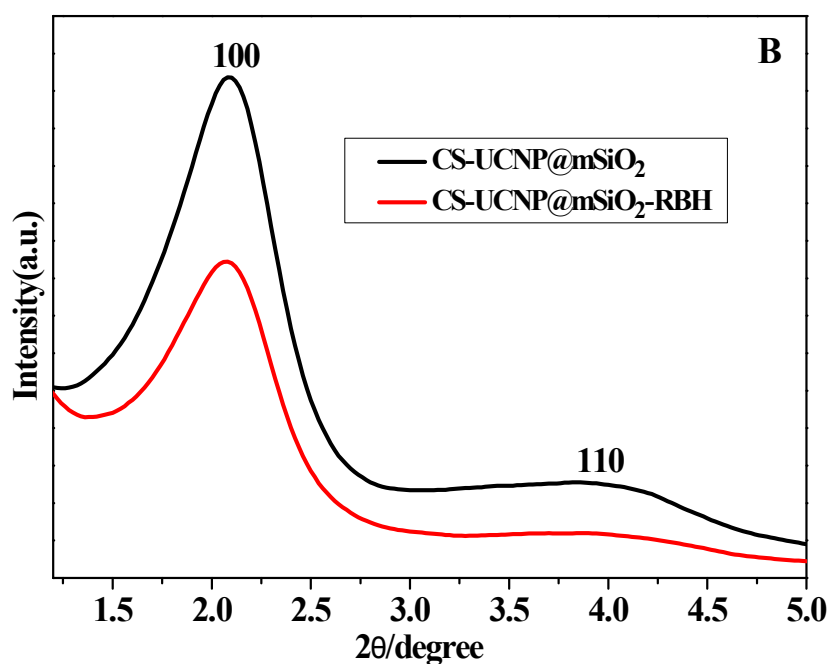
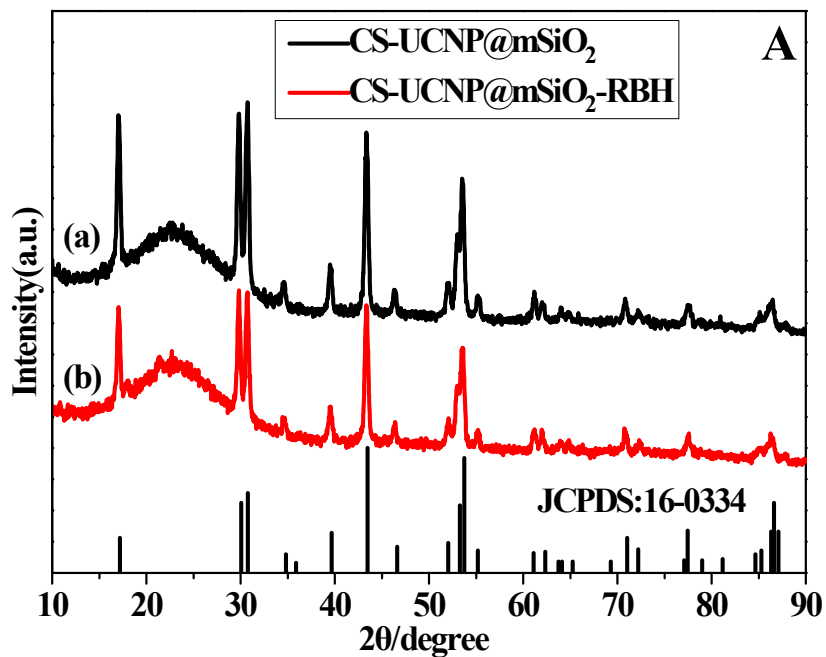


Fig. S2 The X-ray diffraction (XRD) (A) and small-angle X-ray diffraction (SAXRD) (B) patterns of the prepared nanoparticles CS-UCNP@mSiO<sub>2</sub> (a), CS-UCNP@mSiO<sub>2</sub>-RBH (b) and standard pure hexagonal NaYF<sub>4</sub> (JCPDS no.16-0334).

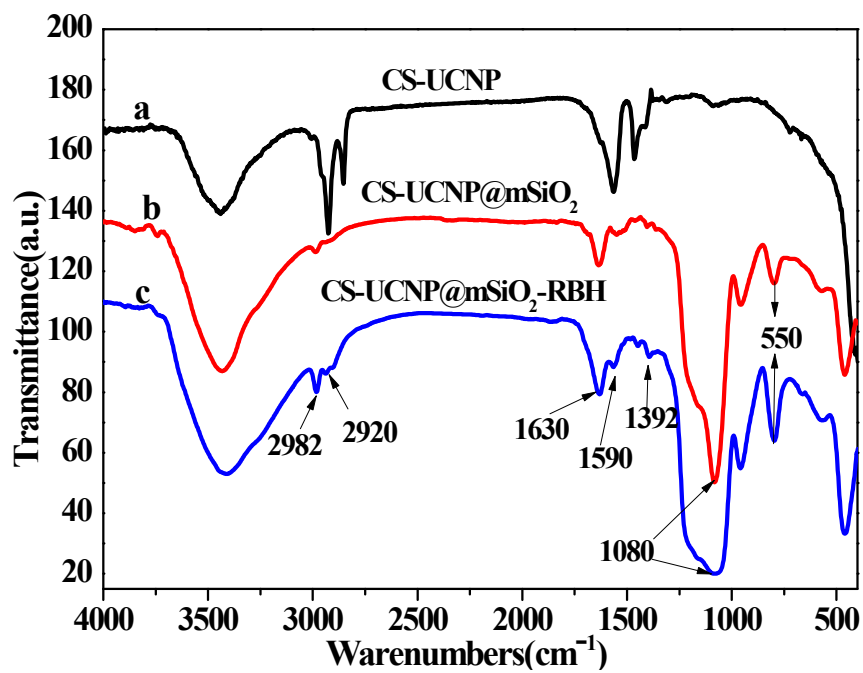


Fig. S3. FTIR spectra of CS-UCNP (a), CS-UCNP@mSiO<sub>2</sub> (b), CS-UCNP@mSiO<sub>2</sub>-RBH(c).

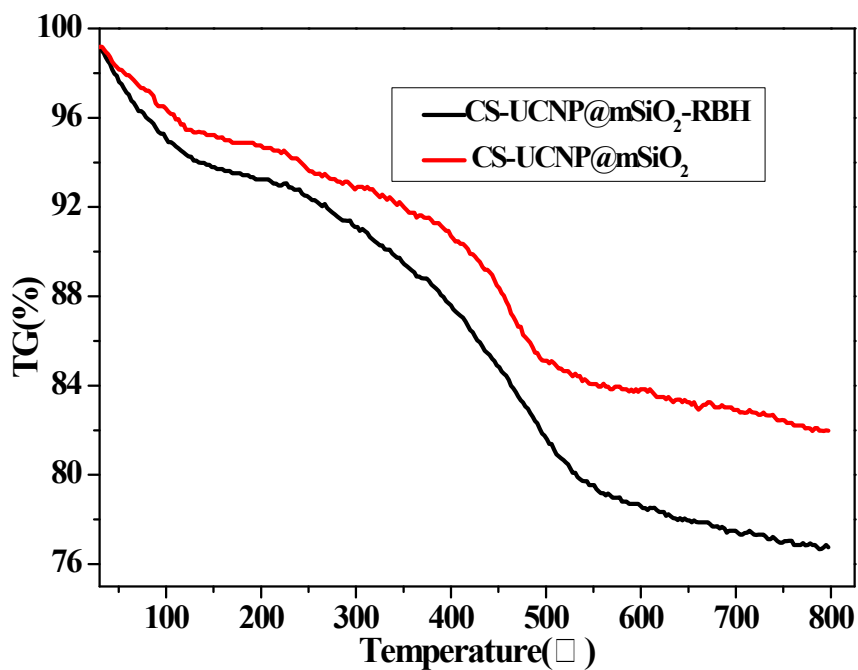


Fig. S4. TG curves of CS-UCNP@mSiO<sub>2</sub> (red curve), CS-UCNP@mSiO<sub>2</sub>-RBH (black curve).

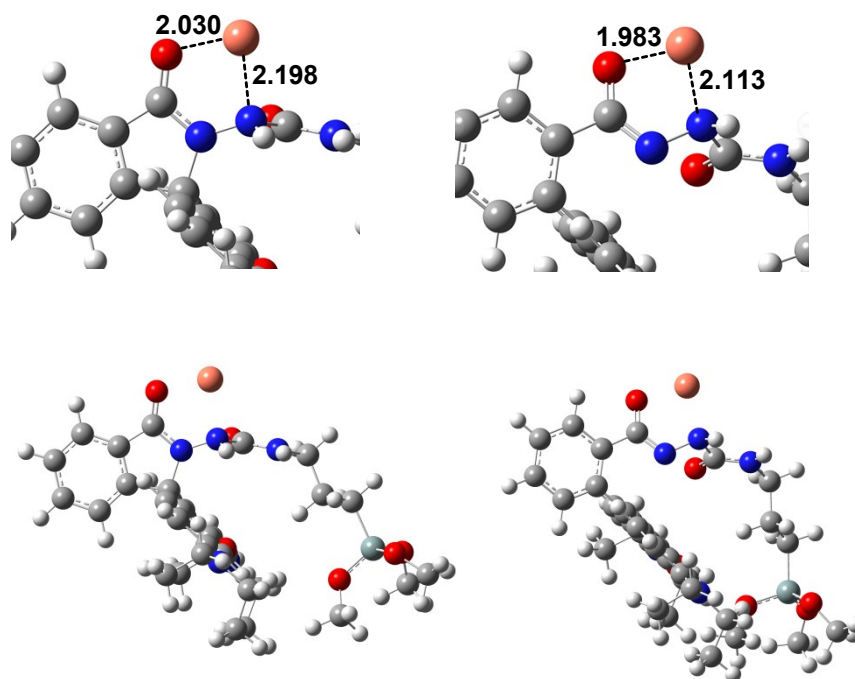
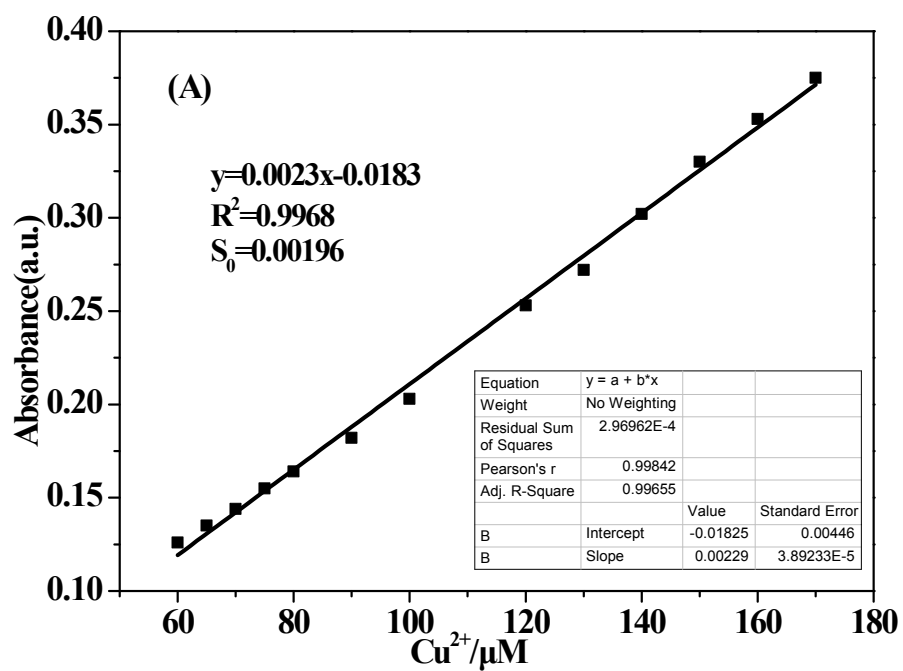


Fig. S5. Optimized  $\text{Cu}^{2+}$  complexes obtained at the B3LYP/[LANL2DZ-ECP/6-31G(d,p)] level of theory.



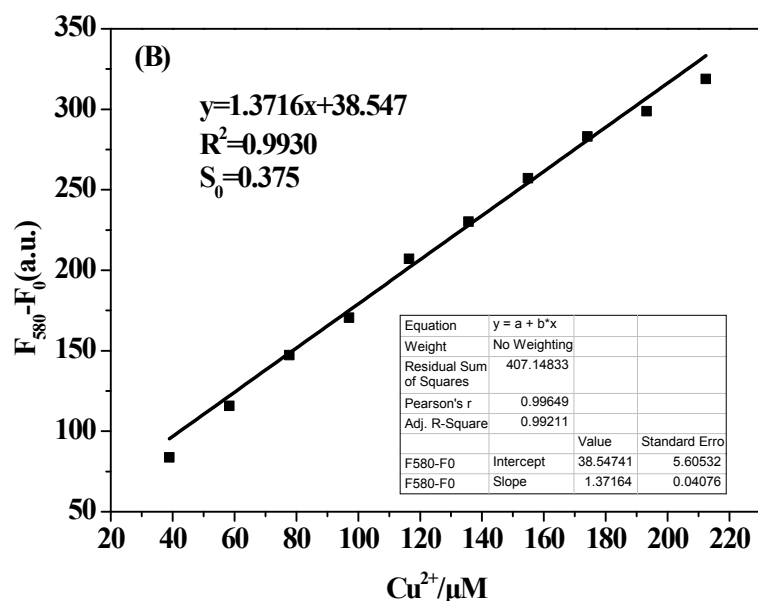


Fig. S6. (A) The absorption intensity at 557 nm of CS-UCNP@mSiO<sub>2</sub>-RBH as a function of Cu<sup>2+</sup> concentrations (60-170 μM). (B) The relative fluorescence intensity at 580 nm of CS-UCNP@mSiO<sub>2</sub>-RBH as a function of Cu<sup>2+</sup> concentrations (40-212 μM).

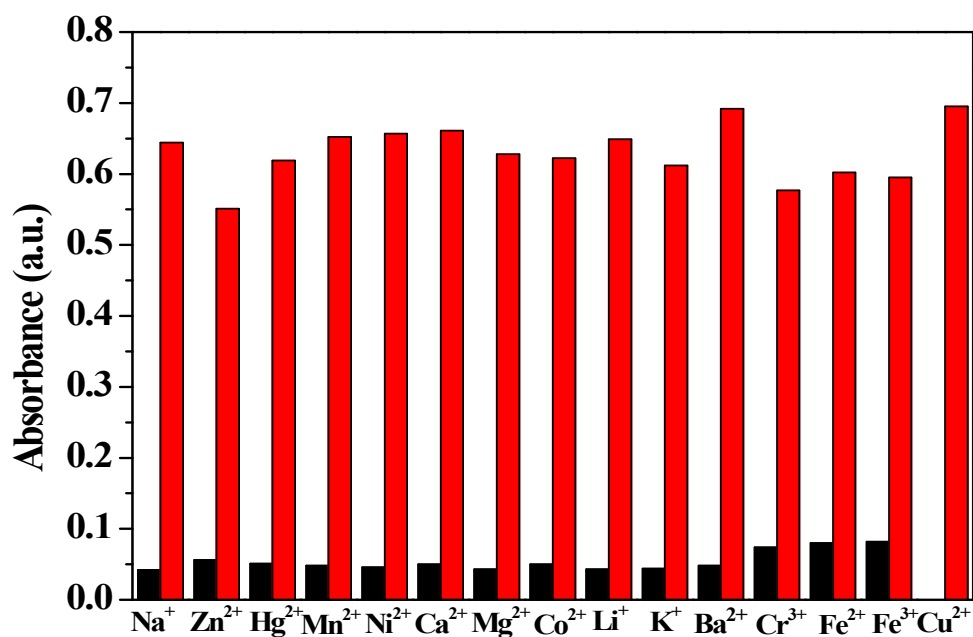


Fig. S7. The absorbance intensity of CS-UCNP@mSiO<sub>2</sub>-RBH in the presence of various cations (0.1 M). The black bars represent the absorbance intensity of CS-UCNP@mSiO<sub>2</sub>-RBH in the presence of various other metal ions. The red bars represent the change of the absorbance upon the subsequent addition of equivalent Cu<sup>2+</sup> to the solution.

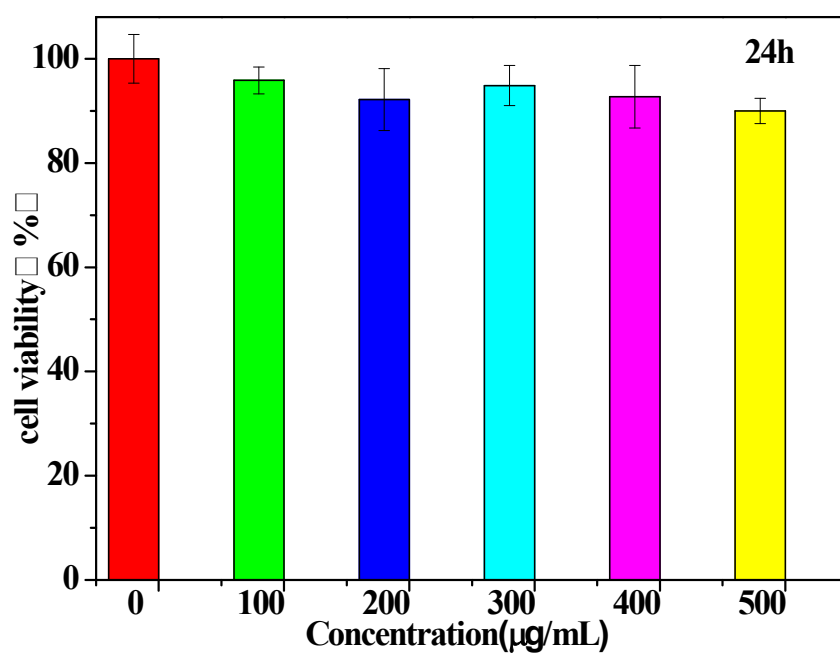


Fig. S8. Percentage of viable HeLa cells after treatment with indicated concentrations of probe CS-UCNP@mSiO<sub>2</sub>-RBH.