

† **Electronic Supplementary Information**

**Rapid, high selective colorimetric detection of mercury (II) ions in
water sources based on ribavirin functionalized AuNPs sensor**

Lvcheng Liu, Yuqi Ling, Junshan Han, Tingting Hao, Xing Li*

School of Materials Science and Chemical Engineering, Ningbo University, Ningbo
315211, China

* Corresponding Authors.

E-mail addresses: lixing@nbu.edu.cn (X. Li).

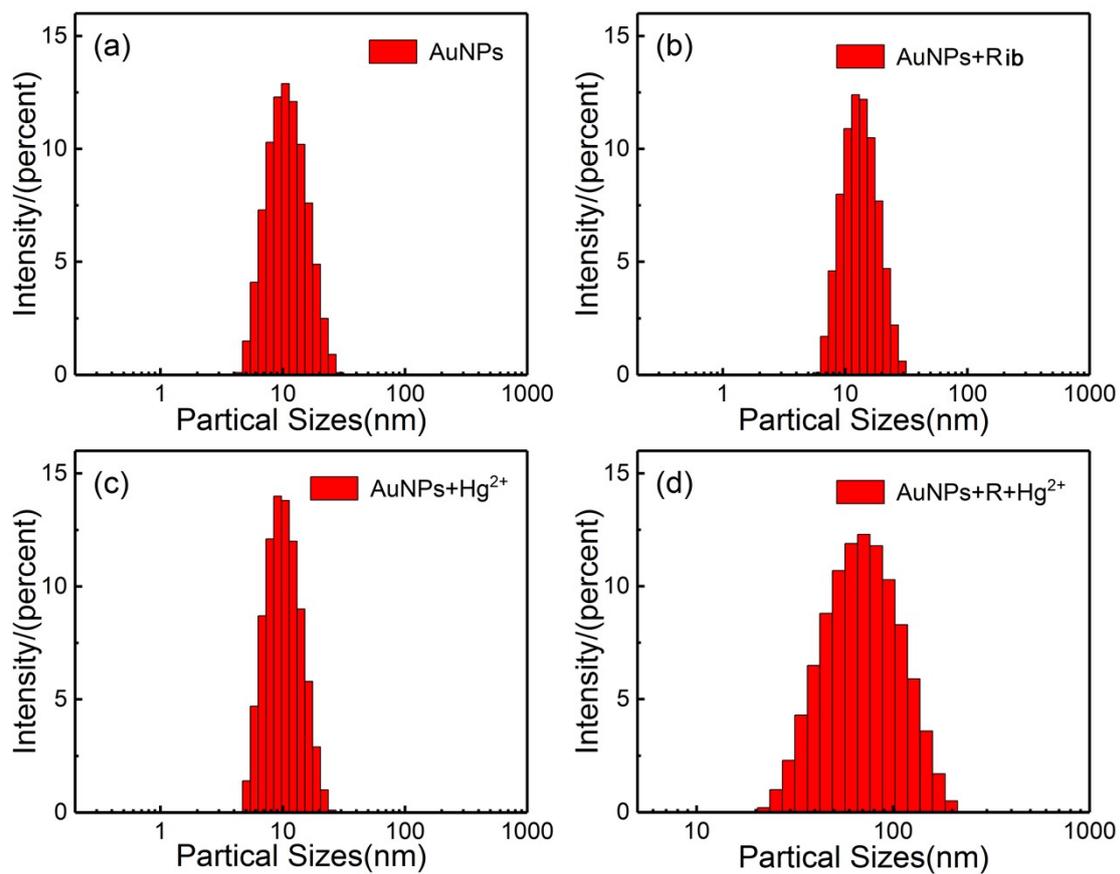


Figure. S1 The DLS results of AuNPs under different additives: **(a)** AuNPs; **(b)** AuNPs with 40mM ribavirin; **(c)** AuNPs with 10 μ M Hg²⁺; **(d)** AuNPs with 40 mM ribavirin in the presence of Hg²⁺ (10 μ M).

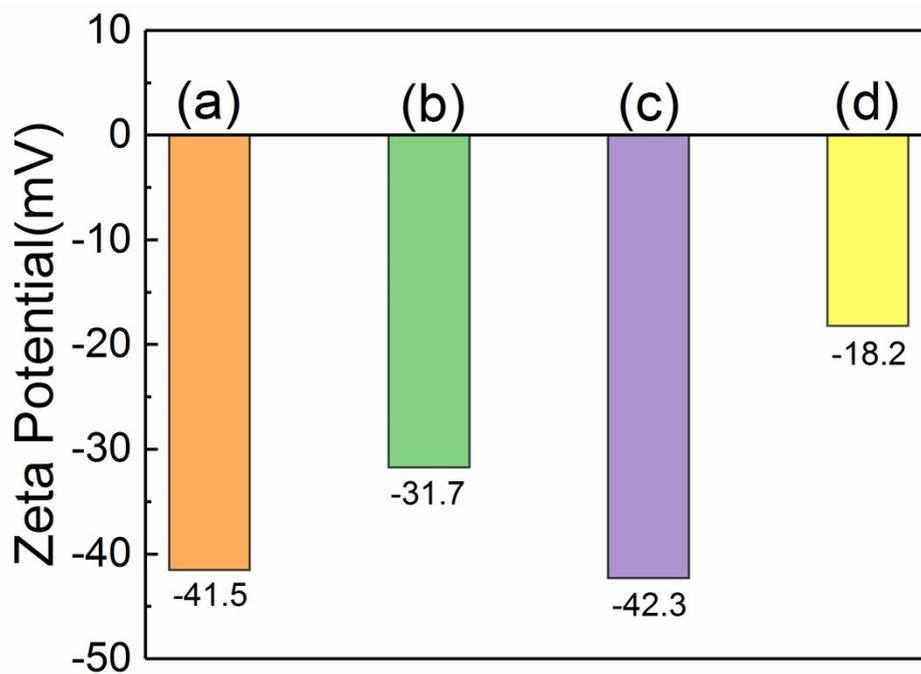


Figure. S2 Zeta potentials of Au NPs under different additives (mV). **(a)** AuNPs; **(b)** AuNPs with 40 mM ribavirin; **(c)** AuNPs with 10 μM Hg^{2+} ; **(d)** AuNPs with 40 mM ribavirin in the presence of Hg^{2+} (10 μM).

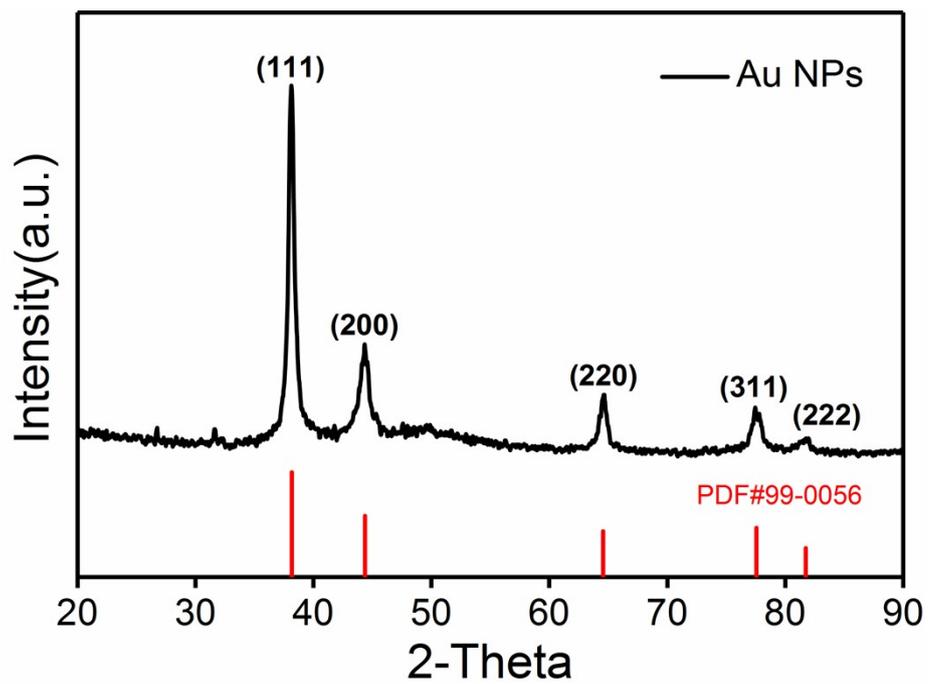


Figure. S3 X-ray powder diffraction patterns of AuNPs in the range of 20 ~ 90°.

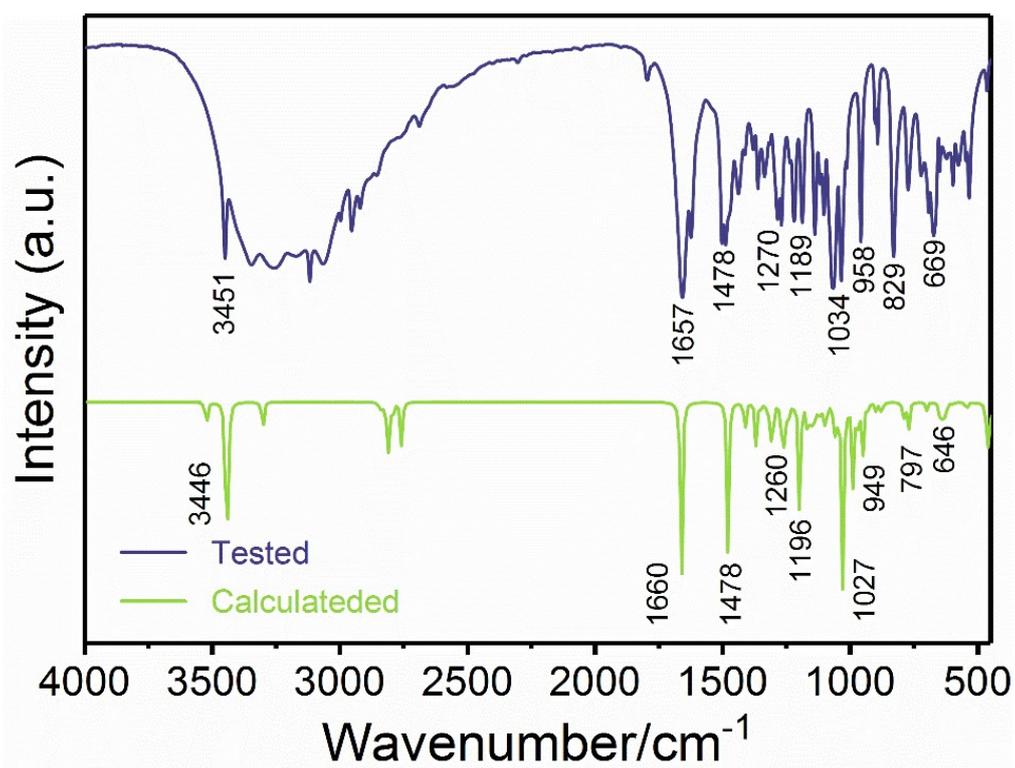


Figure. S4 Fourier transform infrared spectrometry of ribavirin molecular.

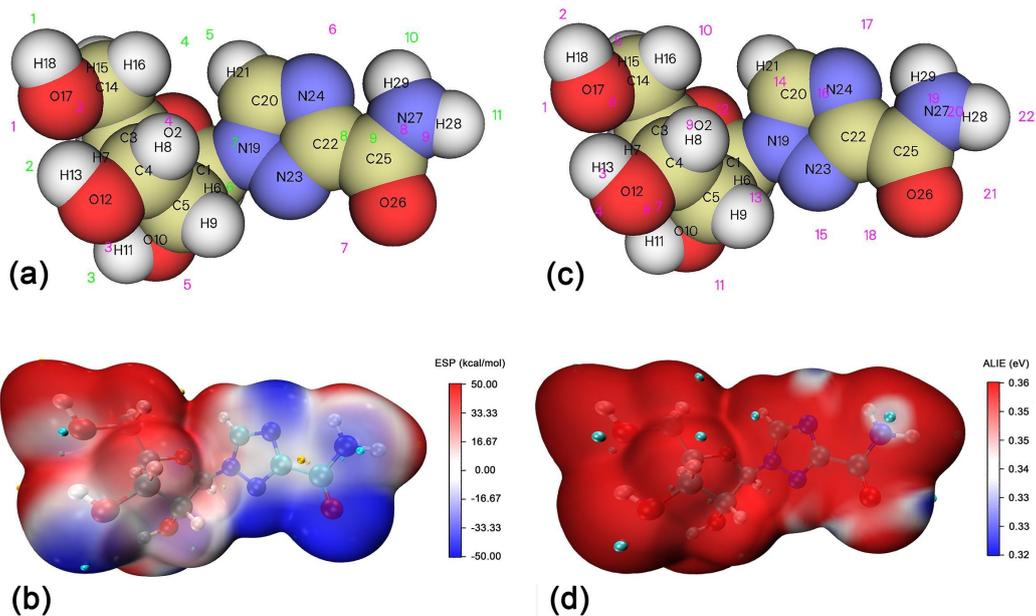


Figure. S5 (a) Distribution diagram of electrostatic potential extreme points on the van der Waals surfaces. (b) Surface electrostatic potentials rendering of ribavirin molecular. (c) Distribution diagram of local ionization energy extreme points on the van der Waals surfaces. (d) Average local ionization energy rendering of ribavirin molecular.

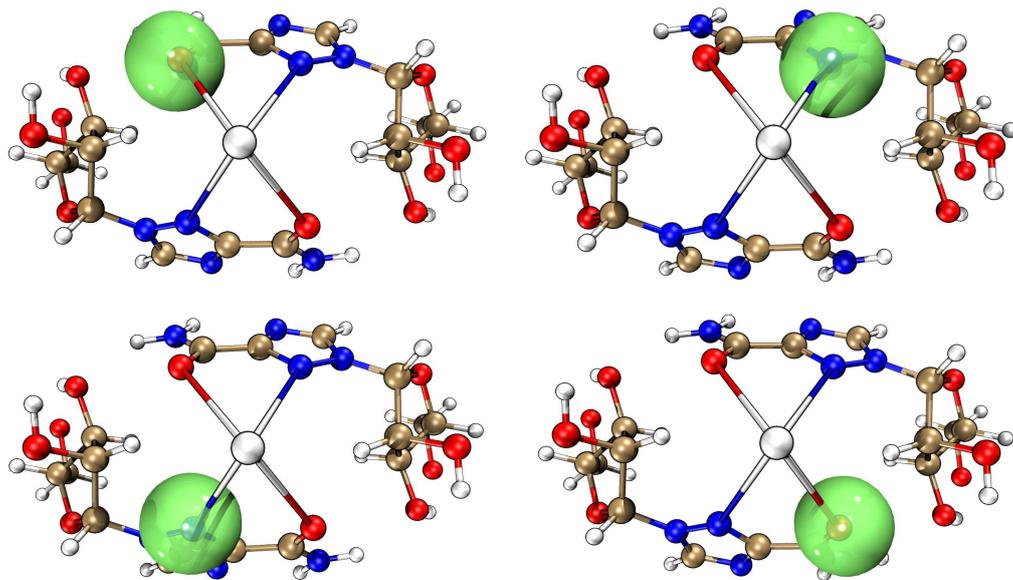


Figure. S6 Partial localized molecular orbitals of $\text{Hg}(\text{ribavirin})_2$.

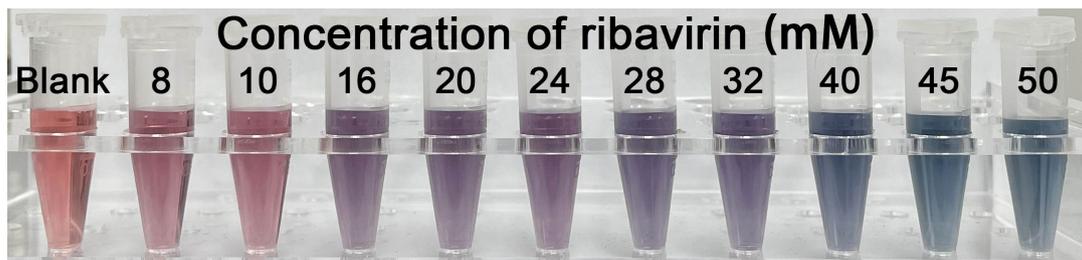


Figure. S7 Optimization of ribavirin concentrations (8, 10, 16, 20, 24, 28, 32, 40, 45 and 50 mM) on the detection of Hg^{2+} by functionalized-AuNPs. The colorimetric images show the detection effect of the colorimetric sensors for Hg^{2+} along with the increase of ribavirins.

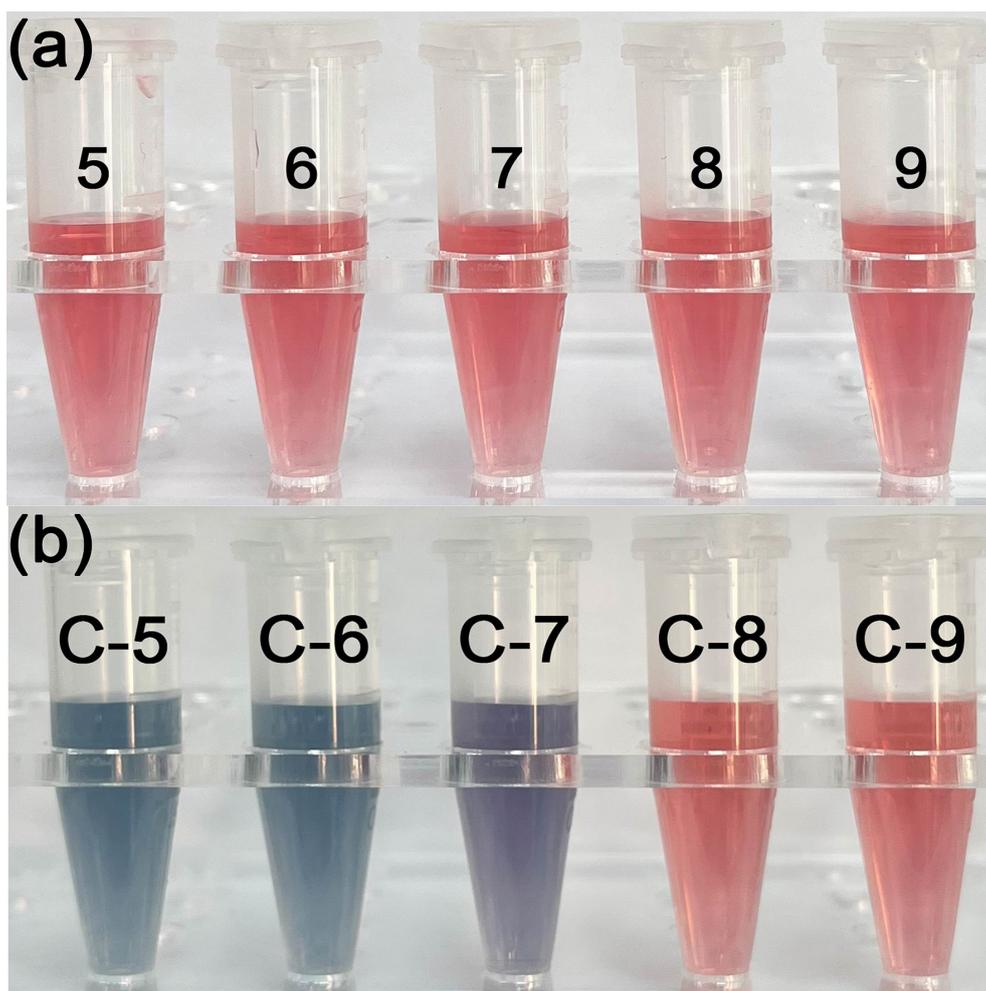


Figure. S8 The effect of pH values (5, 6, 7, 8 and 9) on the detection performances of ribavirins functionalized AuNPs colorimetric sensors for Hg^{2+} : (a) photographs of AuNPs solutions with 40 mM ribavirins under different pH values, (b) photographs of AuNPs solutions with 40 mM ribavirins in the presence of $10 \mu\text{M Hg}^{2+}$ under different pH values.

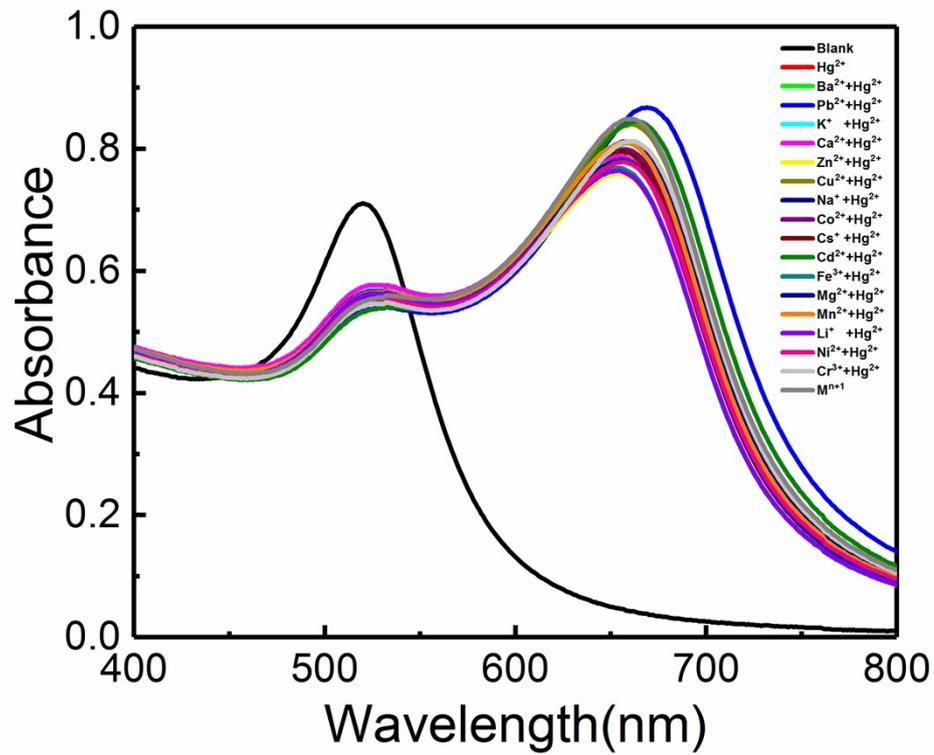


Figure. S9 UV-vis spectra of ribavirin functionalized AuNPs solution in the presence of Hg²⁺ (10.0 μ M) and the mixture of Hg²⁺ and other ions (100 μ M).