

Supporting Information

**Cyclometallated Ruthenium Complex-Modified
Upconversion Nanophosphors for Selective Detection of
Hg²⁺ Ions in Water**

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Figure S1 ¹HNMR spectrum in CD₃CN

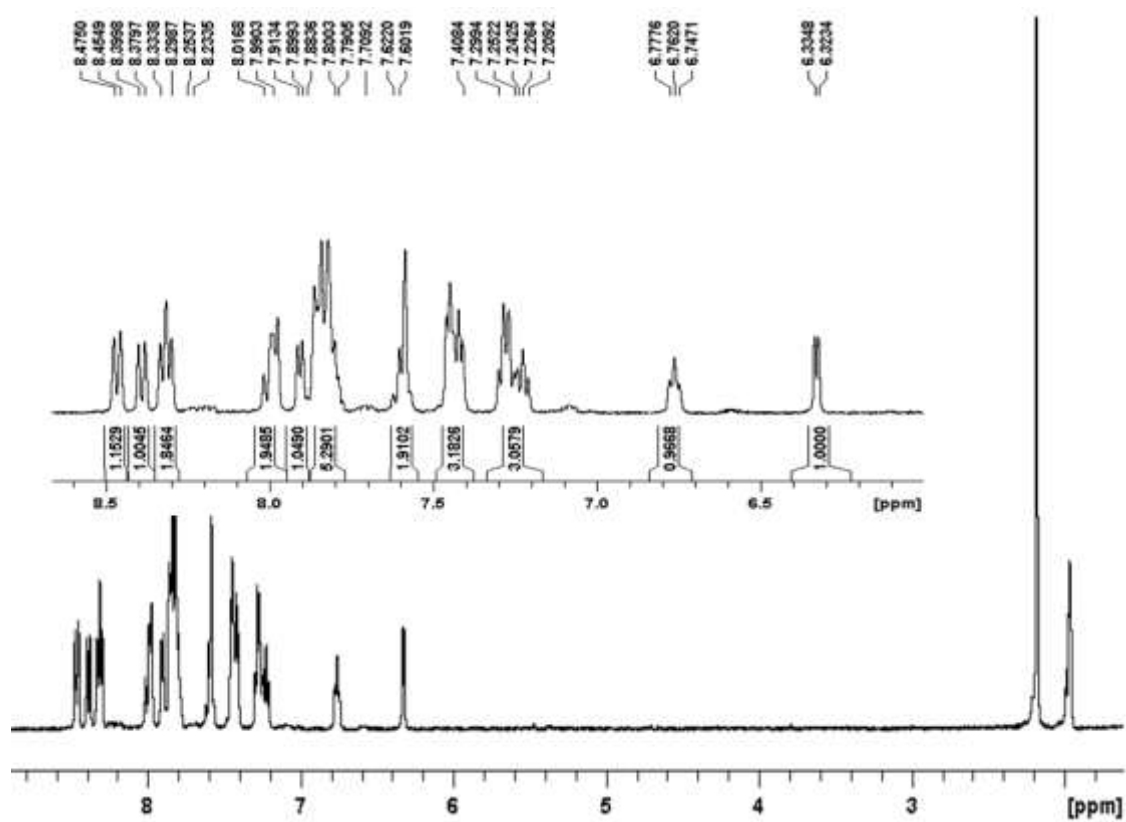


Figure S2 ^{13}C NMR spectrum in CD_3CN

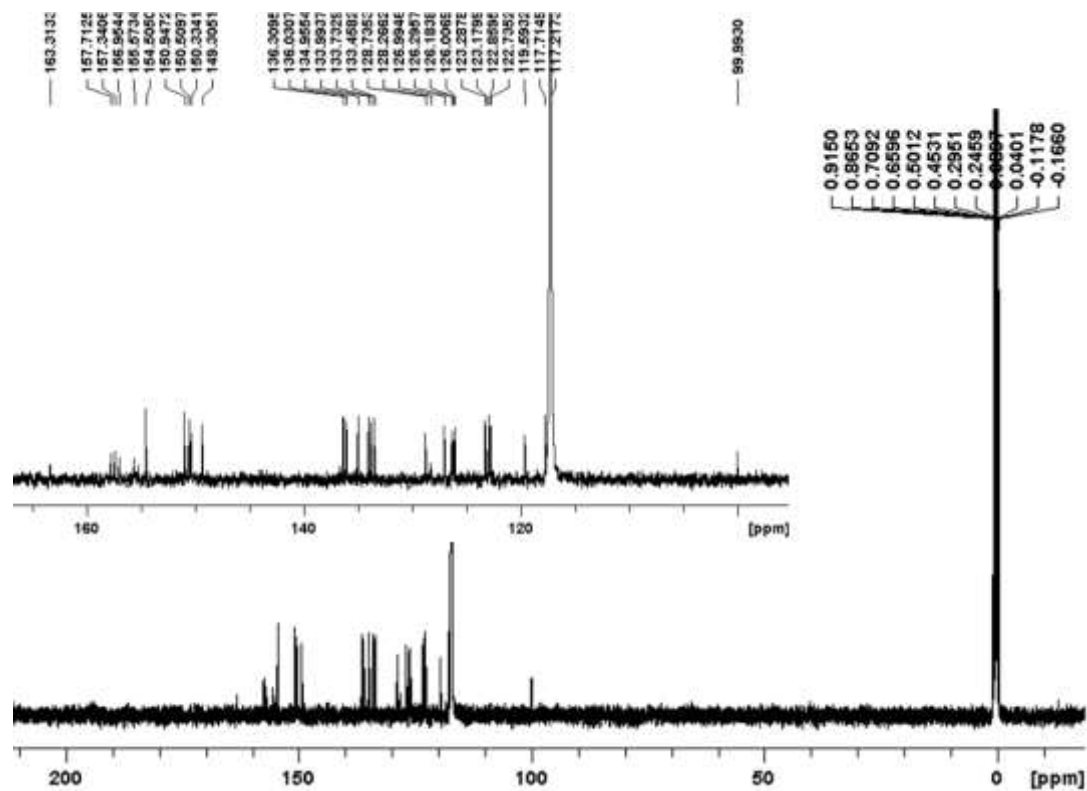


Figure S3 MS spectrum

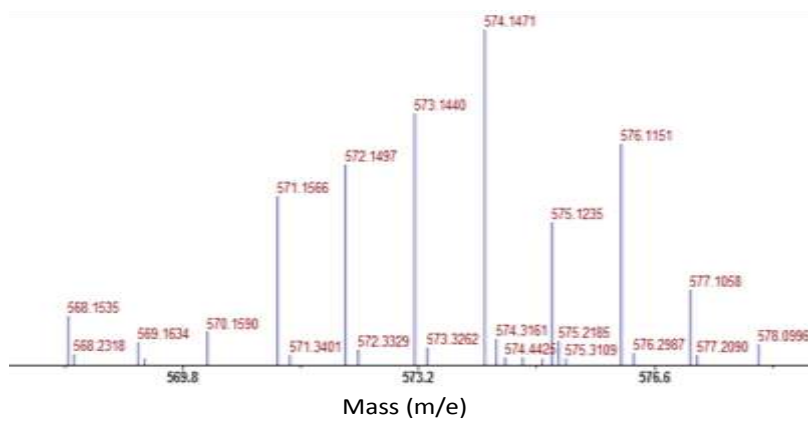


Figure S4 UV-visible response of Ru1 (20 μ M) to various metal ions in CH₃CN solution. Bars represent the absorption intensity $A_{423\text{nm}}/A_{536\text{nm}}$. White bars represent the blank solutions. Black bars represent the addition of metal ions (2 equiv.) to a solution of Ru1.

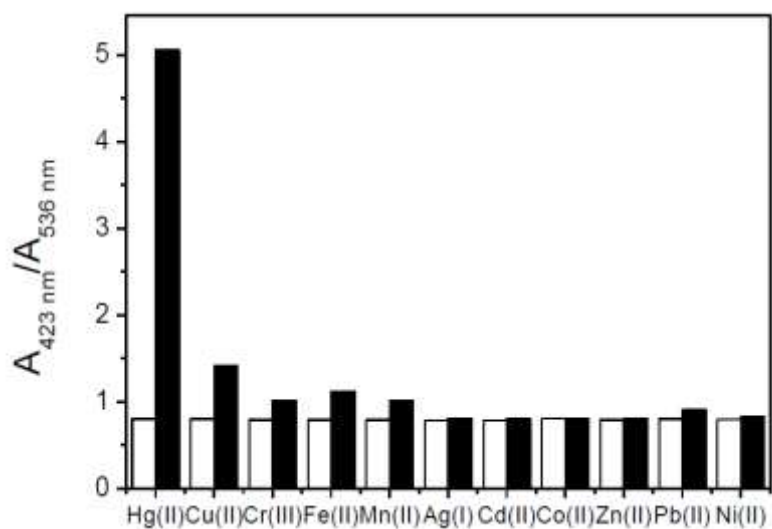


Figure S5 (a) XPS of OA-UCNPs (purple line), PEG-UCNPs (red line), and Ru1-UCNPs in the absence (black line) and presence (blue line) of Hg^{2+} . (b, c) XPS of Ru element in the Ru1-UCNPs.

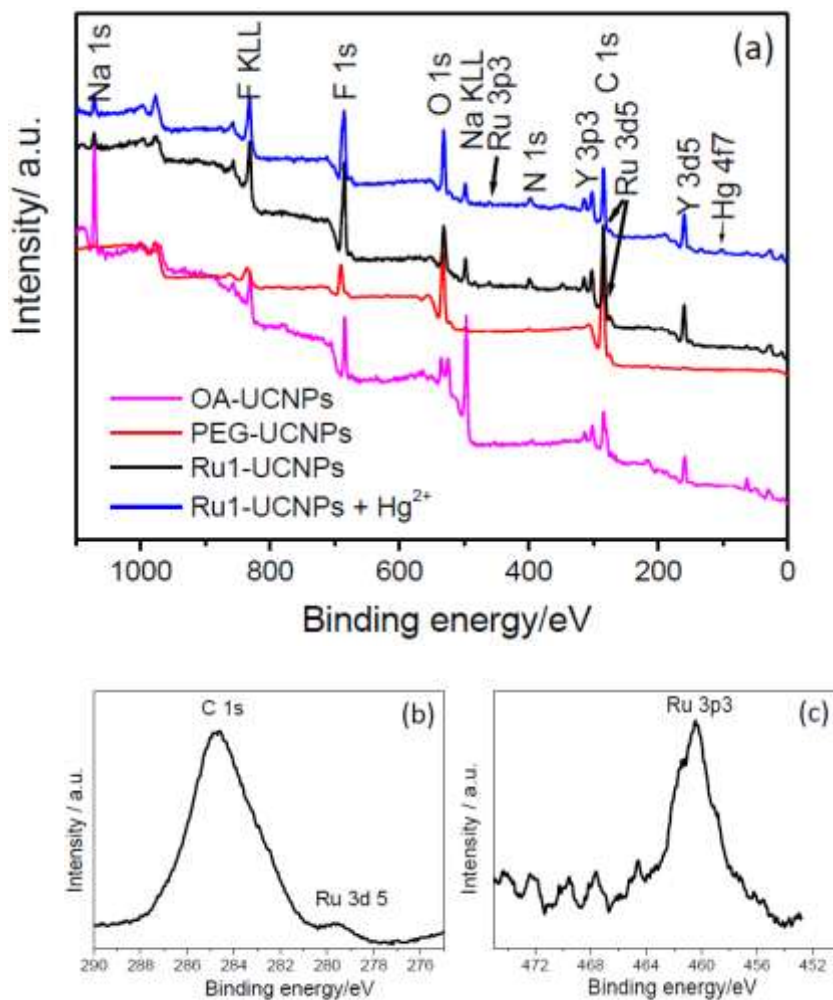


Figure S6 The complex Ru1 concentration of Ru1-UCNPs was calculated using the detailed titration spectra. (a) UV/Vis absorption spectra of Ru1 with different concentrations. (b) The absorbance at 539 nm as a function of Ru1 concentration. The Ru1 content of Ru1-UCNPs was determined as 11.4 wt%. The concentration of Ru1-UCNPs is 0.064 mg/mL.

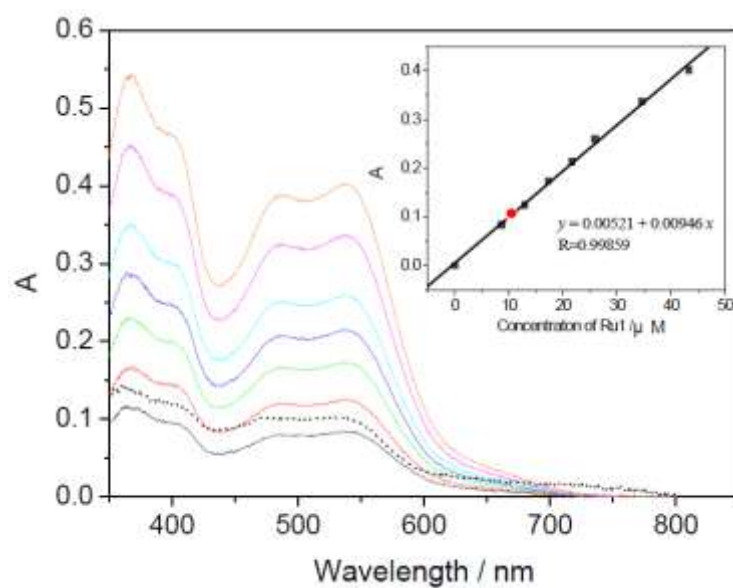


Figure S7. Bright-field and upconversion photographs of Ru1-UCNPs in the presence of 0, 0.3, 0.6, 1.2 equiv. of Hg^{2+} water solutions (10 mM HEPES, pH 7.2).

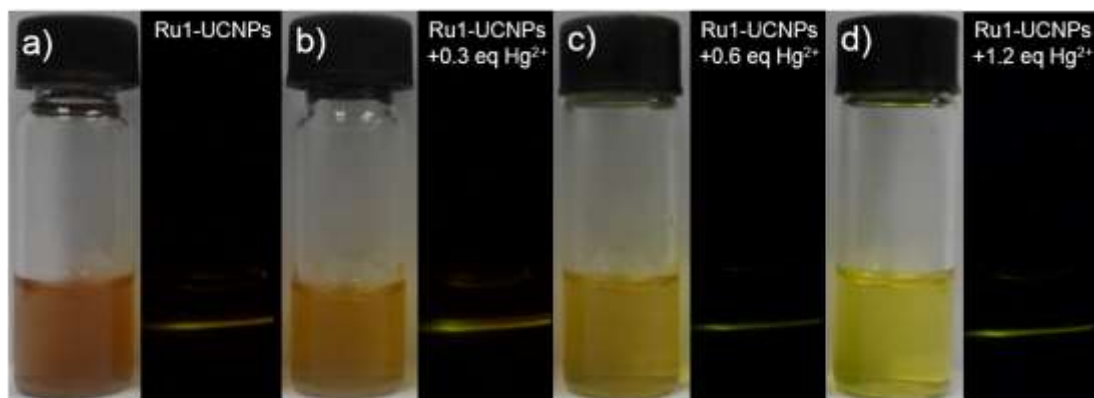
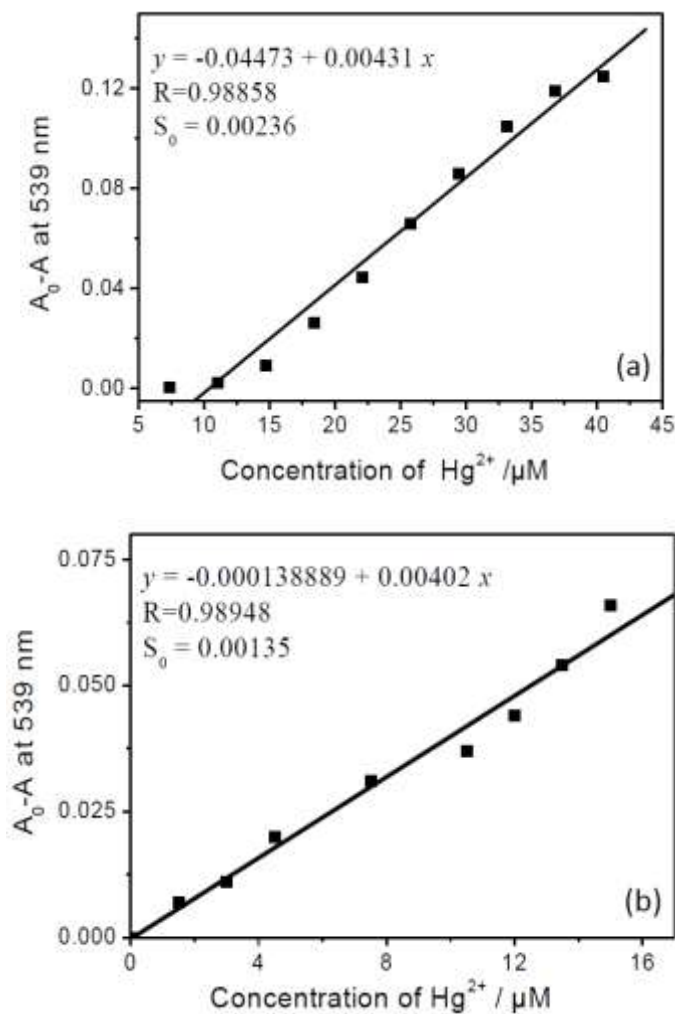


Figure S8. The sensitivity test of Ru1-UCNPs towards Hg^{2+} of Ru1 (a) and Ru1-UCNPs (b) using UV/Vis absorption technique. (c) The sensitivity test towards Hg^{2+} of Ru1-UCNPs using upconversion luminescence emission technique. The detection limit (LOD) was given by the equation $\text{LOD} = 3S_0/S$; where 3 is the factor at the 99% confidence level, S_0 the standard deviation of the blank measurements, and S is the slope of the calibration curve. The limit of detection (LOD) was determined to be 329, 200, and 8.2 ppb of Hg^{2+} , respectively, for Ru1 (a) and Ru1-UCNPs (b) using UV/Vis absorption technique and for Ru1-UCNPs using UCL emission technique.



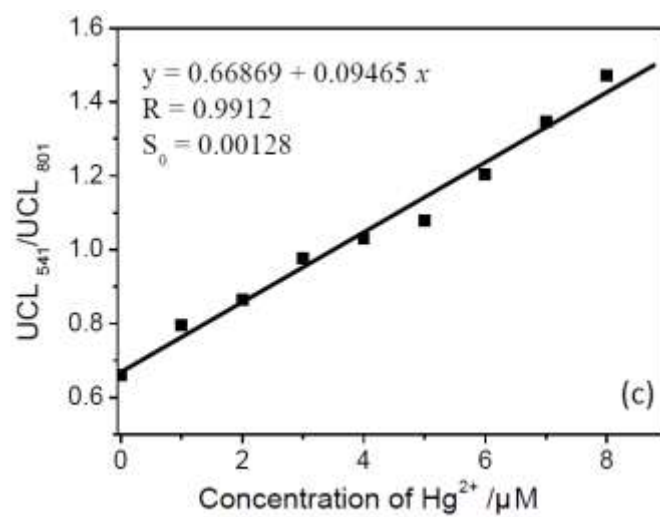


Figure S9. Ru1-UCNPs stored in water solution (10 mM HEPES, pH 7.2) for 3 days. Photographs of Ru1-UCNPs solution before (a) and after (b) centrifugation. (c) Corresponding absorption spectra of the sample in the upper solution after centrifugation. The control sample is the solution containing free Ru1 molecules with the same concentration as in the Ru1-UCNPs nanocomposite.

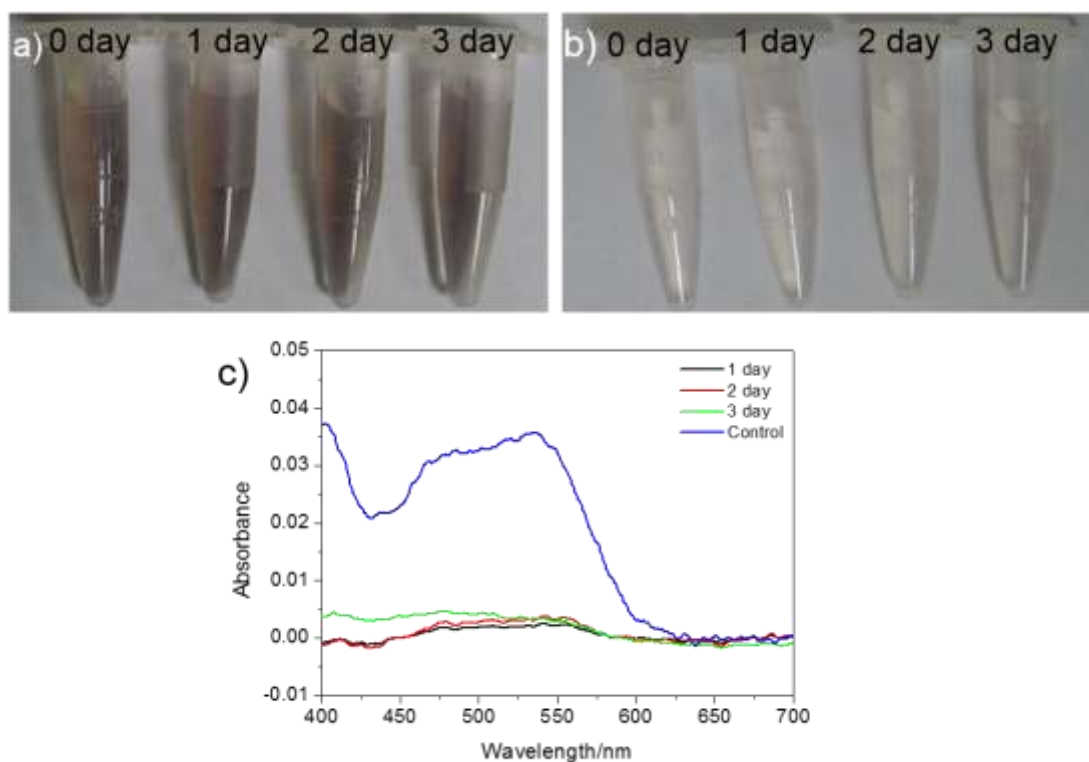


Figure S10. Bright-field and upconversion emission photographs of Ru1-UCNPs in the presence of mixed metal cations (Pb^{2+} , Cu^{2+} and Fe^{2+}) (a), and with addition of 1.2 equiv. of Hg^{2+} (b) in water solutions (10 mM HEPES, pH 7.2). (c) Corresponding photoluminescence spectra of the Ru1-UCNPs with an excitation wavelength $\lambda = 980$ nm.

