

Supporting information
**Ligand engineering of luminescent AuAg
nanoclusters for targeted mitochondria and brain
imaging**

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Experimental

Chemicals and Materials.

Ultrapure water (18.2 M Ω ·cm) was used in the whole experiment. Hydrogen tetrachloroaurate(III) hydrate (HAuCl₄·3H₂O), silver nitrate (AgNO₃), GSH (\geq 99%), EDC (\geq 98%), NHS (\geq 98%), 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) was purchased from Sigma-Aldrich. Sodium hydroxide (NaOH), and TPP were ordered from Sinopharm Chemical Reagent Co., Ltd. Phosphate buffer solution (PBS) was purchased from Qingdao Hope BioTechnology Co., Ltd. Hoechst 33342, and MitoTracker® Green FM were ordered from Invitrogen (Carlsbad, CA).

Instrumentation.

Transmission electron microscope (TEM) images of samples were obtained with a JEOL JEM 2100F microscope with an operating voltage of 200 kV. UV-visible absorption and luminescence spectra were acquired on a Shimadzu UV-1800 spectrophotometer and a PerkinElmer FL-8500 fluorescence spectrometer, respectively. The luminescence decay results were collected on a photoluminescence spectrometer (FLS-1000, Edinburgh Instruments Ltd.). X-ray photoelectron spectra (XPS) were recorded on an Axis Ultra DLD X-ray photoelectron spectrometer using a standard Al K α X-ray source. The binding energy of the C 1s level of adventitious carbon at 284.8 eV was used for energy calibration. The surface chemistry of samples was analyzed by a Fourier transform infrared spectrometer (FTIR, Nicolet iS10). Thermogravimetric analysis (TGA) was conducted on a NETZSCH TG209F1 system with a heating rate of 10 °C min⁻¹ under an air atmosphere. Zeta potential was obtained

by using a Zetasizer Nano ZS (Malvern Co., England). Hemoatoxylin/eosin (H&E) stained images were taken on an inverted fluorescence microscope (OLYMPUS IX73).

Cells culture.

Mouse microglia cells (BV2 for short, American Type Culture Collection, ATCC, Manassas, VA) and mouse breast cancer cells (4T1 for short, American Type Culture Collection, ATCC, Manassas, VA) were cultured in dulbecco's modified eagle medium (DMEM) supplemented with 10 % FBS (fetal bovine serum) and 1 % P/S (penicillin/streptomycin) in an atmosphere of 5 % CO₂ and 95 % air at 37 °C.

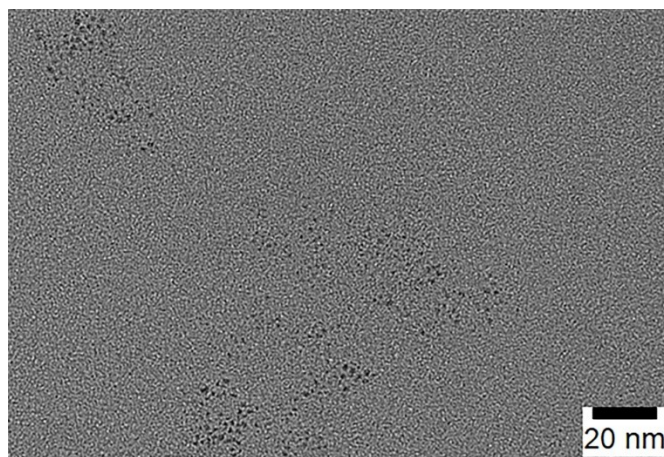


Fig. S1 A representative TEM image of the GSH-protected AuAg NCs.

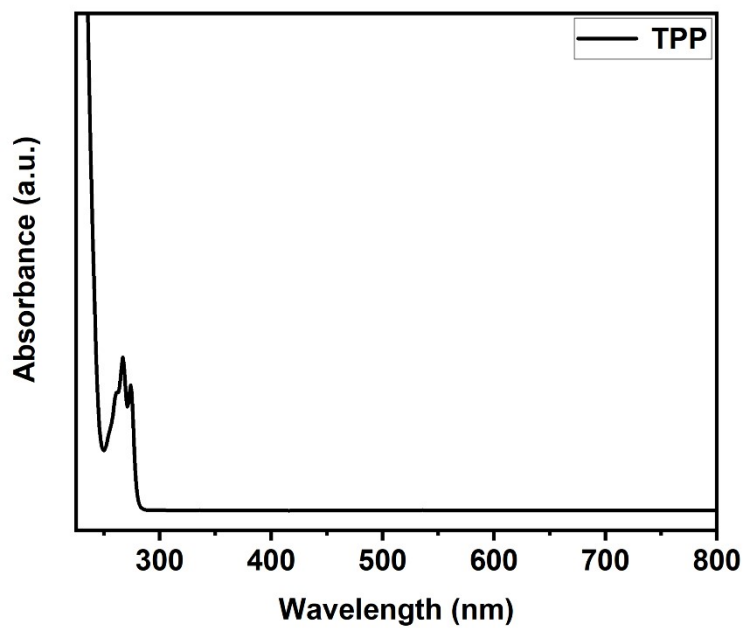


Fig. S2 UV-visible absorption spectrum of the TPP solution.

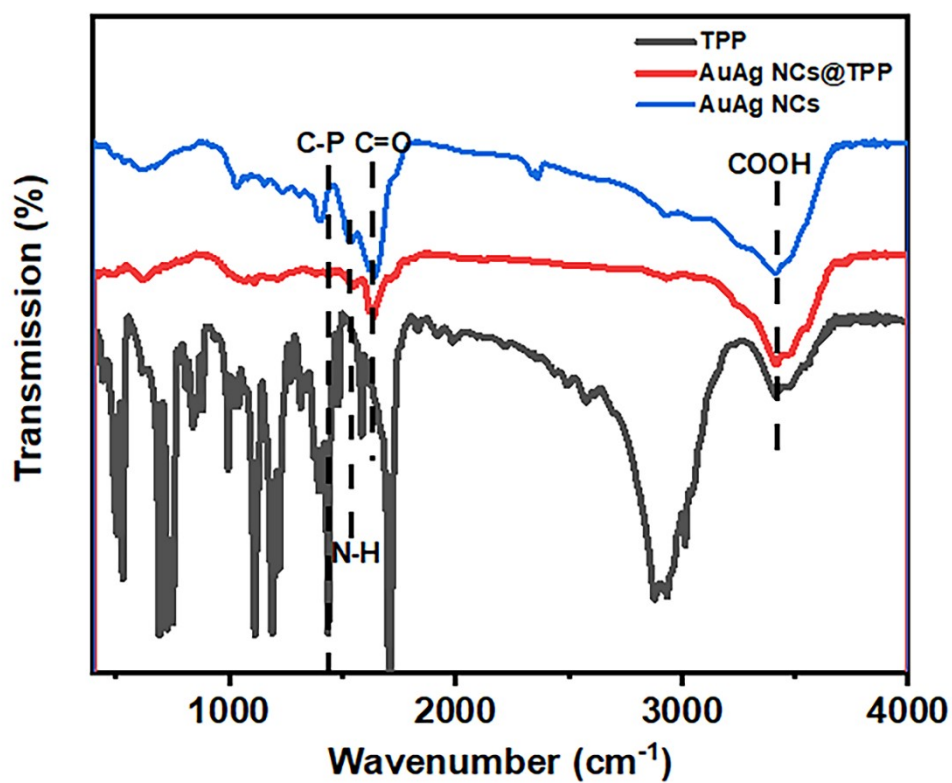


Fig. S3 FTIR spectra of pristine AuAg NCs, AuAg NCs@TPP and TPP.

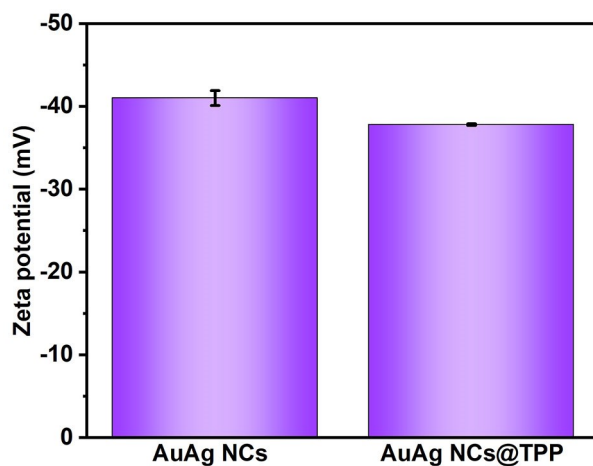


Fig. S4 Zeta potentials of AuAg NCs and AuAg NCs@TPP.

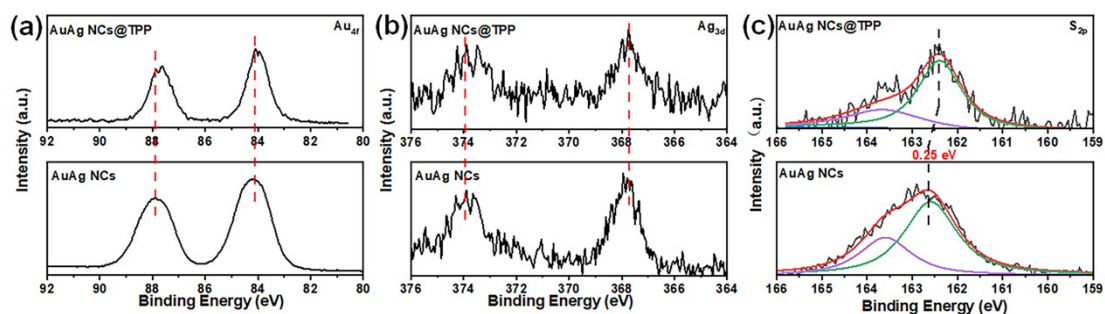


Fig. S5 High-resolution XPS spectra of (a) Au_{4f} , (b) Ag_{3d} and (c) S_{2p} components in the AuAg NCs@TPP and pristine AuAg NCs.

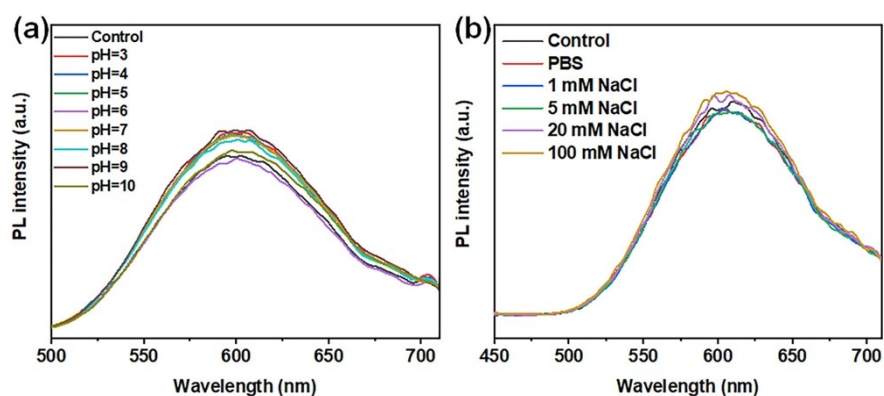


Fig. S6 PL spectra of the AuAg NCs@TPP in (a) solutions with different pH values (ranging from 3 to 10) for 24 hours, and (b) PBS or saline solutions with different NaCl concentrations (i.e., 1, 5, 20, and 100 mM) for 24 hours.

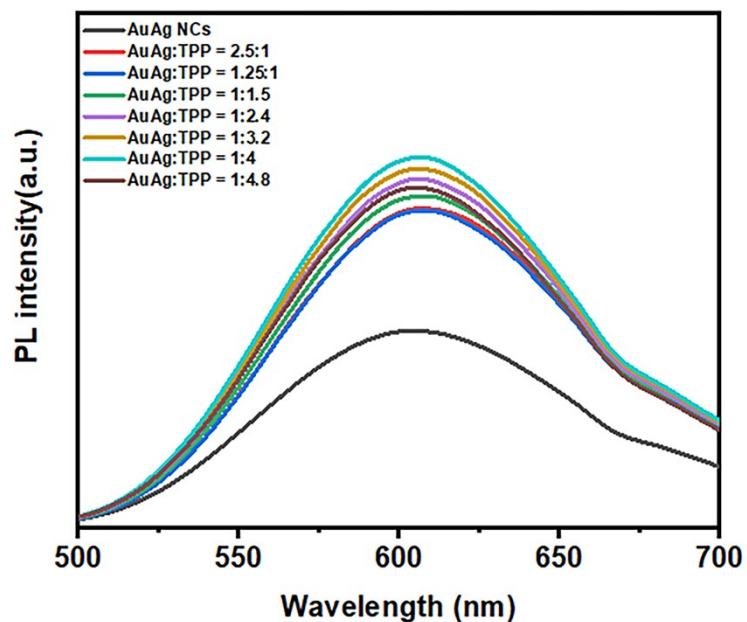


Fig. S7 PL spectra of the AuAg NCs@TPP with different feeding molar ratios of AuAg ions to TPP.

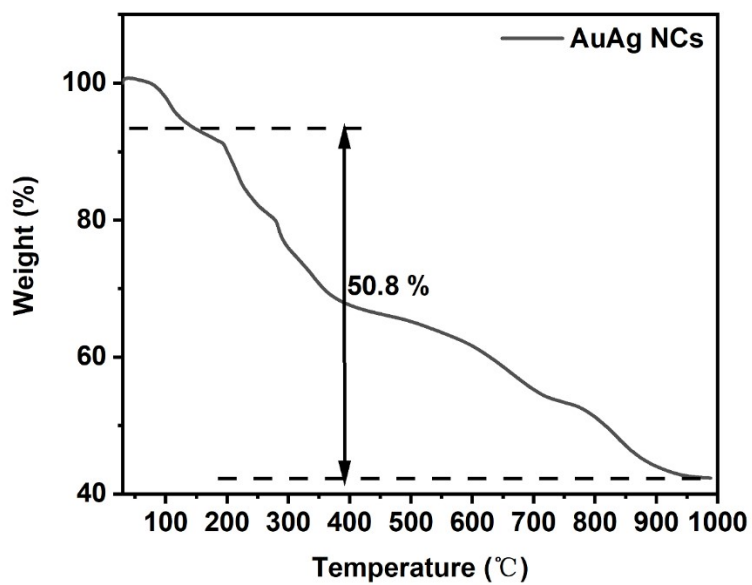


Fig. S8 The TGA curve of AuAg NCs.

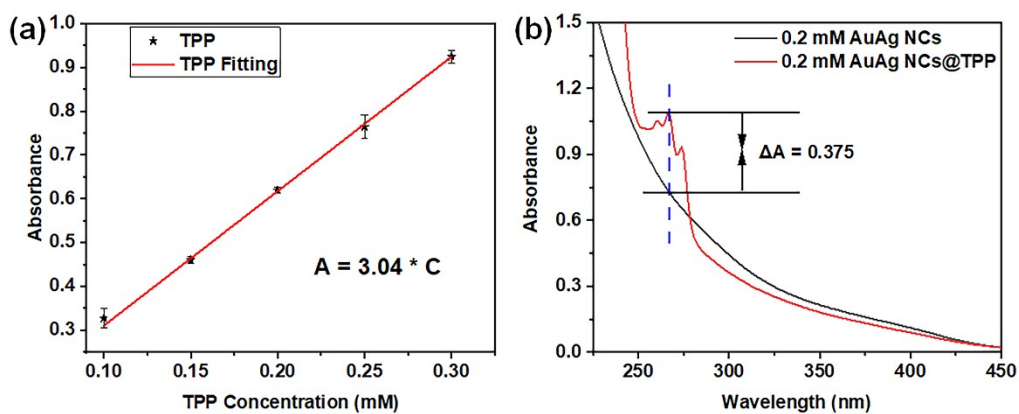


Fig. S9 (a) The linear correlation between the absorbance and the concentration of TPP; (b) The comparison in the absorbance between pristine AuAg NCs and AuAg NCs@TPP at 267 nm.

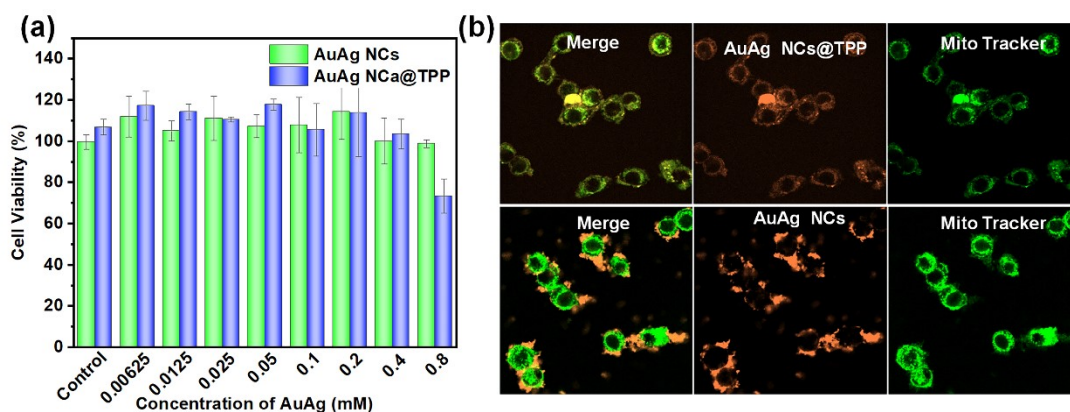


Fig. S10 (a) In vitro cytotoxicity of AuAg NCs@TPP and pristine AuAg NCs for BV2 cells; (b) Confocal PL images of BV2 cells co-stained with Mito-tracker and AuAg NCS@TPP or AuAg NCs (0.4 mM).

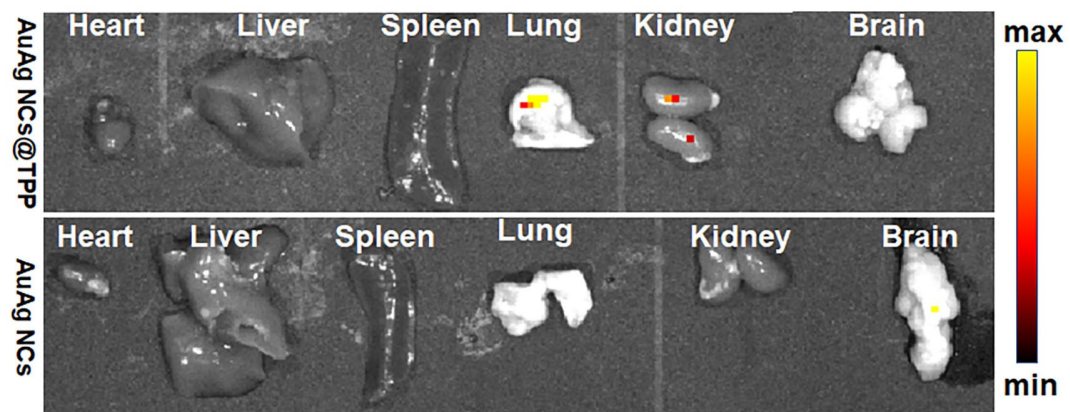


Fig. S11 The bio-distribution of AuAg NCs@TPP and pristine AuAg NCs in heart, liver, spleen, lung, kidney, and brain 10 days after intravenous injection.