Electronic Supplementary Information (ESI)

One-pot synthesis of β-cyclodextrin modified gold nanocluster with near-infrared emission

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EXPERIMENTAL SECTION

Chemicals and Apparatus. Tetrachloroauric acid trihydrate ($HAuCl_4 \cdot 3H_2O$) was purchased from Beijing Huawei Ruike Ltd. The monothiol-modified β-cyclodextrin(β-SH-CD) was purchased from Beijing Huawei Ruike Ltd. All reagents were used without secondary purification. The experiment used water as secondary distilled water.

The emission spectrum was detected by HORIBA Fluoromax-4 fluorescence spectrophotometer, and the PTI-QM4 steady-stead fluorescence spectrophotometer was equipped with R928 PMT and InGaAs photodetectors (75 W xenon arc lamp); UV-visible absorption spectrum was determined by Shimadzu UV-2600 spectrophotometer detection; Lifetime was detected by Techcomp FLS900 transient optical lifetime detector; Transmission electron microscope spectrum was detected by JEOL JEM-2100 high-resolution transmission electron microscopy at an acceleration voltage of 100 kV, and the sample was prepared through two sample droplets provided by Zhongxingbairui Technology Co., Ltd. Carbon film covering ultra-thin copper nets for sample preparation; Raman spectrum detected by Iuvia Refl Raman spectrometer; infrared spectrum detected by Nicolet 6700 infrared spectrometer; XPS spectrum detected by Thermo Fisher-ESCALAB 250Xi X-ray photoelectron spectrometer.

Synthesis of AuNCs@β-CD with near-infrared emission. $NaHCO_3$ (200.00 mg, 2.38 mmol) was dissolved in H_2O (25.0 mL) to prepare an alkaline reaction solution and a concentration at around 0.1 M. β-SH-CD (69.04 mg, 0.06 mmol) solution was dissolved in 1.96 mL of $NaHCO_3$ aqueous solution to prepare β-SH-CD alkaline reaction solution. After adding an aqueous solution of $NaHCO_3$ (40μL, 1M) of tetrachloroauric acid trihydrate to a 25 mL round bottom flask, and 1.04 mL of an aqueous $NaHCO_3$ solution was added at room temperature. Under vigorous stirring, the β-SH-CD alkaline reaction solution was added dropwise. With the addition of β-SH-CD alkaline reaction solution, the color of the mixed solution immediately changed from yellow to colorless. After adding 22 mL of $NaHCO_3$ aqueous solution, it was quickly transferred to an oil bath, and heated at 80°C for 24 h. The color of the mixed solution gradually changed from colorless to pink, and finally to light brown-red. The reaction was stopped, and after returning to room temperature, it was filtered with a 200-mesh aqueous filter to obtain a light brown-red aqueous solution. The solution was then added to a 10 KDa ultrafiltration centrifuge tube and centrifuged at 7,500 rpm to obtain the product. The product is stored at low temperature. The preparation method in the optimization experiment is the same, and only the corresponding parameters are changed.

SUPPLEMENTARY FIGURES

Table S1. Calculation of quantum yield of AuNCs@β-CD ("Sample" and "ref" stand for AuNCs@β-CD and Rhodamine 6G (standard samples); QYref is the quantum yield of rhodamine 6G at 25°C in ethanol).

Samples	*A*sample (at 450 nm)	*A*ref (at 450 nm)	*F*sample	*F*ref	*η*sample	*η*ref	*QY*ref	*QY*sample
AuNCs @β-CD	0.039	0.042	52392485	2278700705	1.33	1.36	0.98	0.02001

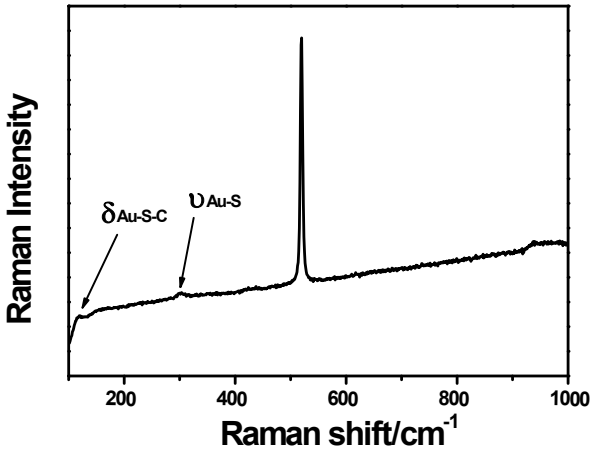

Figure S1. Raman spectrum of AuNCs@β-CD.

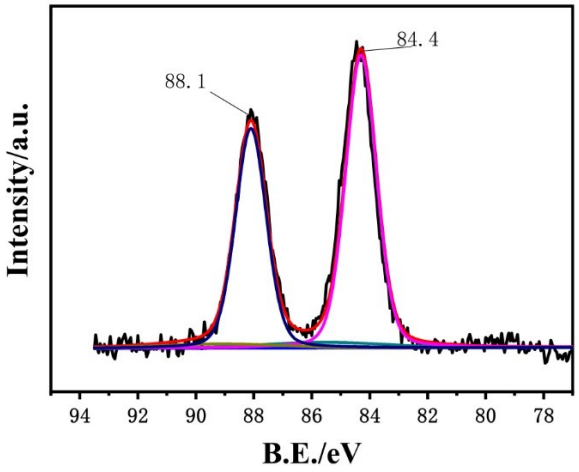

Figure S2. XPS spectra of the AuNCs@β-CD (Au 4f).

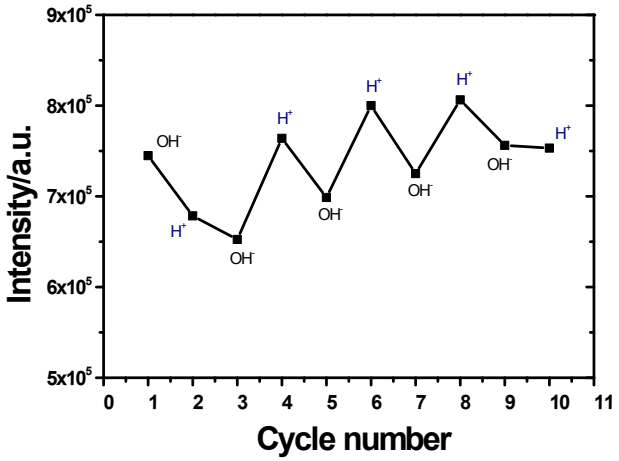

Figure S3. Effect of pH on the photoluminescent intensity of AuNCs@β-CD after preparation (λ_{ex} = 450 nm; λ_{em} = 795 nm; AuNCs concentration is 2×10^{-3} M; back and forth between pH = 2 and pH = 9).

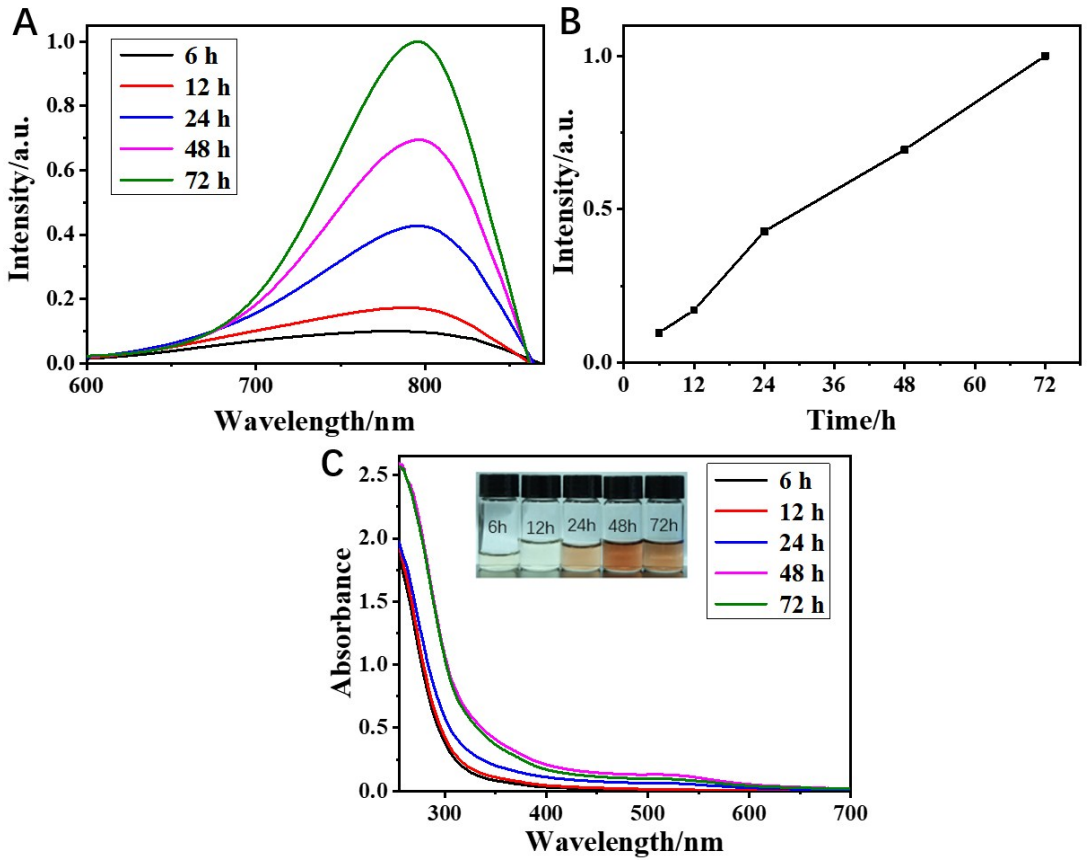

Figure S4. (A) Photoluminescence spectra of AuNCs@β-CD by different preparation time as well as (B) its variation trend of intensity, and (C) the UV-Vis absorption spectra, Inset: The picture of AuNCs@β-CD in aqueous solution under sunlight.

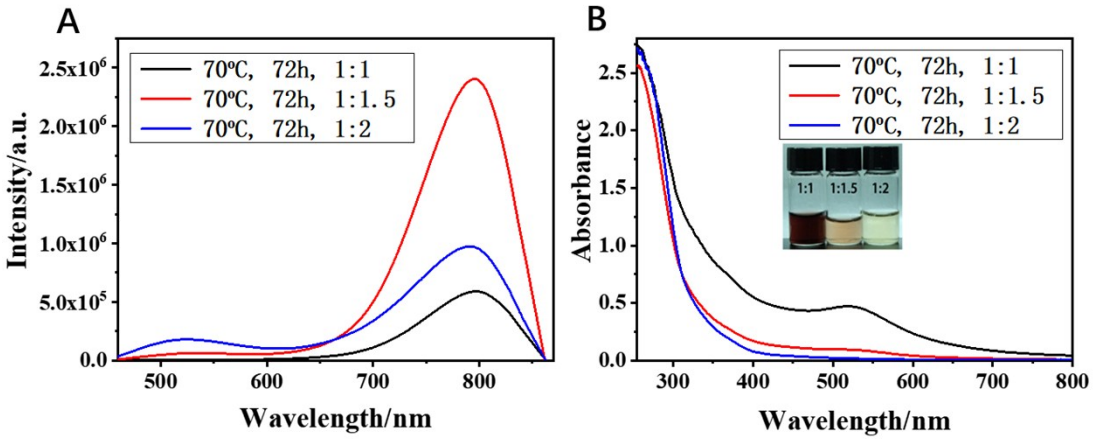

Figure S5. (A) Photoluminescence spectra of AuNCs@β-CD by different ratios of Au/SH as well as (B) its UV-Vis absorption spectra, Inset: The picture of AuNCs@β-CD in aqueous solution under sunlight.

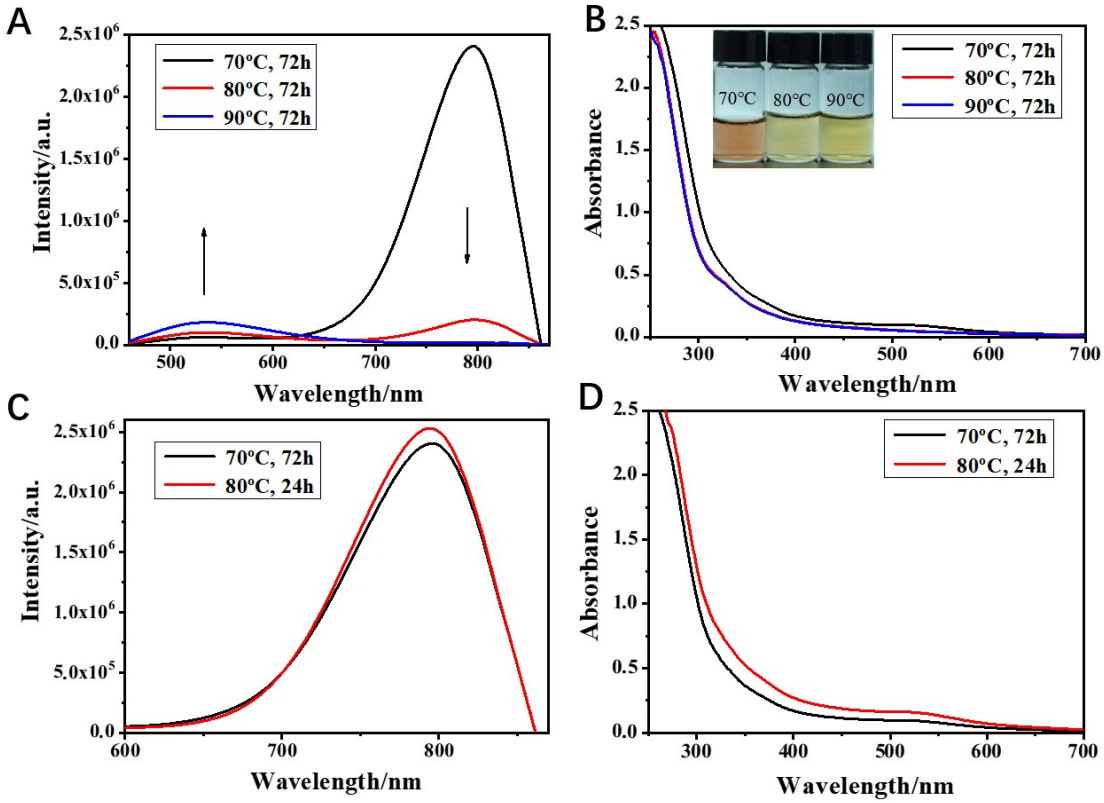

Figure S6. (A) Photoluminescence spectra of AuNCs@β-CD by different preparation temperature as well as (B) its UV-Vis absorption spectra, Inset: the picture of AuNCs@β-CD in aqueous solution under sunlight. (C) The photoluminescence spectra of AuNCs@β-CD with close intensity obtained by two preparation methods; (D) and its UV-Vis absorption spectra.