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Supporting Information

pH-induced reversible self-assembly of gold nanoparticles functionalized with self-complementary zwitterionic peptides for near-infrared photothermal antibacterial treatment

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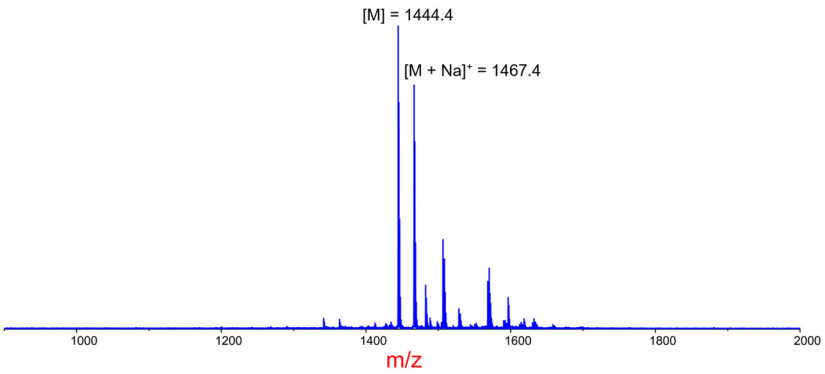

Fig. S1 (a) MALDI-TOF-MS spectrum of ZP. The calculated mass is 1444.4. The highest peak is at 1444.4 = $[M]^+$. The second highest peak is at 1467.4 = $[M+Na]^+$. The matrix we used is 2,5-dihydroxybenzoic acid (DHB) and the test was performed in reflection mode.

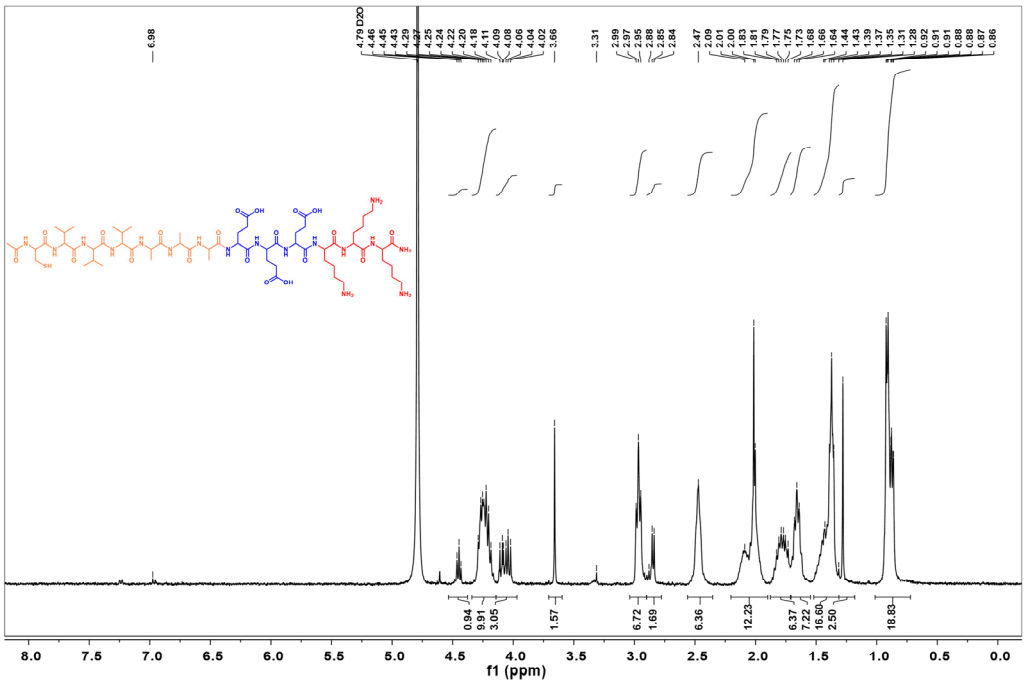

Fig. S2 ^{1}H NMR spectrum (400 MHz, D_2O) of ZP.

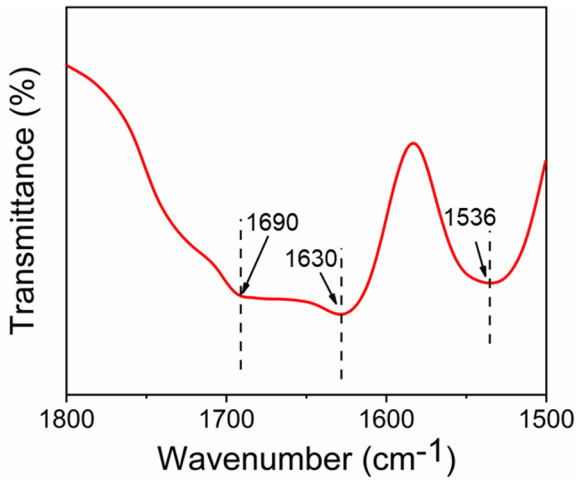

Fig. S3 ATR-FTIR spectrum of ZP assemblies in aqueous solution.

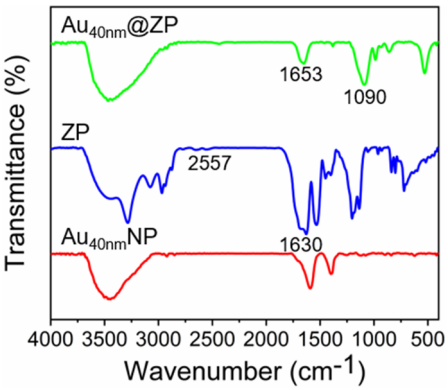

Fig. S4 FTIR spectra of $Au_{40nm}NP$, ZP and Au_{40nm}@ZP. The characteristic band of free thiol at 2557 of the ZP spectrum disappeared in Au_{40nm}@ZP due to their conjugation with AuNPs. The N-H bending and C-O stretching at 1653 cm^{-1} and 1090 cm^{-1} in Au_{40nm}@ZP implied successful conjugation of ZP with $Au_{40nm}NP$, attributable to the amide groups of the ZP.[1, 2]

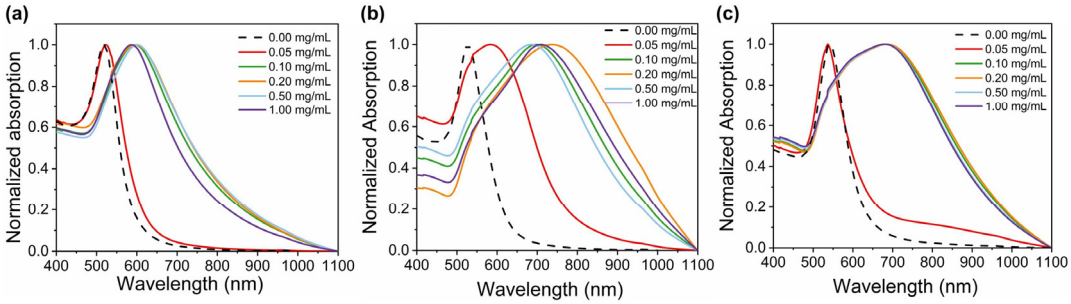

Fig. S5 UV-vis spectroscopy of AuNPs@ZP with the various amounts of ZP addition, $AuNP_{15nm}$@ZP (a), $AuNP_{40nm}$@ZP (b) and $AuNP_{60nm}$@ZP (c).

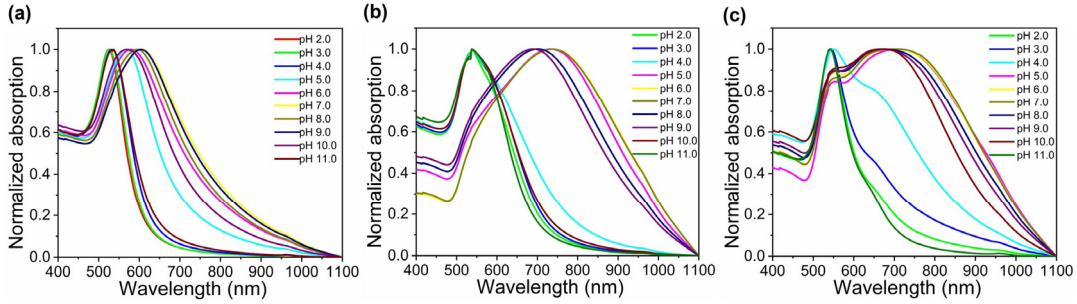

Fig. S6 UV-vis spectroscopy of AuNPs@ZP at various pH values, $AuNP_{15nm}$@ZP (a), $AuNP_{40nm}$@ZP (b) and $AuNP_{60nm}$@ZP (c).

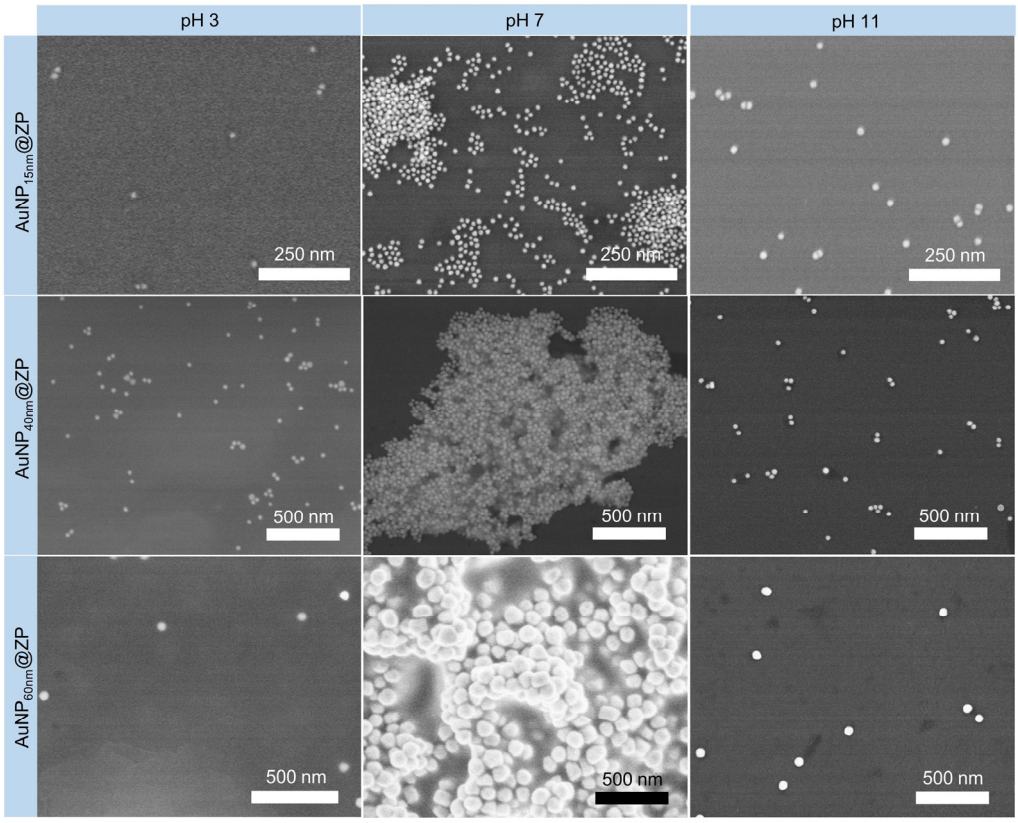

Fig. S7 SEM images of AuNPs@ZP at pH 3, 7 and 11, respectively.

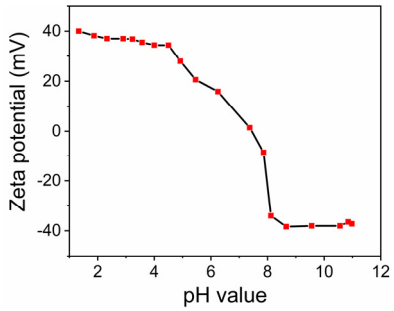

Fig. S8 The zeta potentials of AuNP$_{40nm}$@ZP at different pH values.

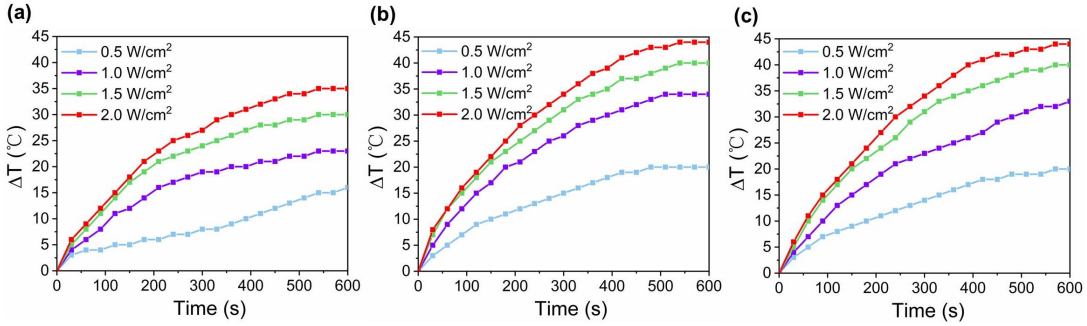

Fig. S9 The photothermal performance of AuNPs@ZP was related to the laser power density, AuNP$_{15nm}$@ZP (a), AuNP$_{40nm}$@ZP (b) and AuNP$_{60nm}$@ZP (c) (150 μg/mL).

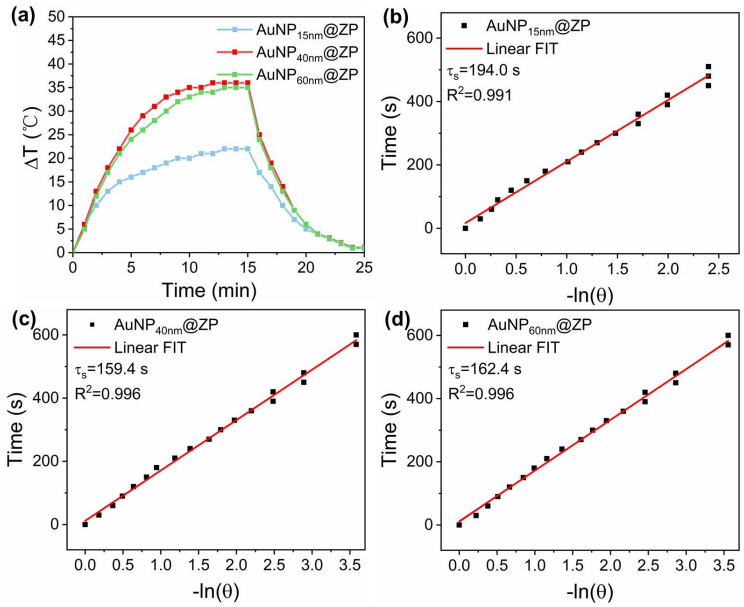

Fig. S10 The photothermal conversion efficiency of AuNPs@ZP. (a) The temperature elevation of AuNPs@ZP aqueous solutions (200 μL) irradiated with 1.0 W·cm^{-2} NIR for 15 min and turned off for 10 min. (b-d) Linear time data versus -lnθ obtained from the cooling period of the aqueous solution, AuNP$_{15nm}$@ZP (b), AuNP$_{40nm}$@ZP (c) and AuNP$_{60nm}$@ZP (d), respectively. The photothermal conversion efficiency calculated is 22.7%, 32.8% and 27.9%, respectively.

1 S. Mohebbi, T. Tohidi Moghadam, M. Nikkhah and M. Behmanesh, *Nanoscale Res Lett*, 2019, **14**, 13.
2 S. S. Sankari, H. U. Dahms, M. F. Tsai, Y. L. Lo and L. F. Wang, *Colloids Surf B Biointerfaces*, 2021, **208**, 112117.