Supplementary Material (ESI) for Chemical Communications


*Supporting Information for:*

# Peptide-tailored assembling of Au nanorods

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## Experimental section

**Chemicals and reagents.** Sodium borohydride ($NaBH_4$), chlorauric acid ($HAuCl_4 \cdot 3H_2O$), cetyltrimethylammonium bromide (CTAB), silver nitrate ($AgNO_3$), L-ascorbic acid (AA), and 4-mercaptopyridine (4MP) were all purchased from Alfa Aesar and used as received. Peptides with various amino acid sequences such as oxidized glutathione (GS-SG), P13 (SVRGWYVRSVFDP), P15 (DELERRIRELEARIK), P16 (AEAEAKAKAEAEAKAK) and P21 (EPYNEWTLELLEELKSEAVRH) are purchased from Shanghai. Milli-Q water (18MΩ.cm) was used for all solution preparations.

**Gold nanorods synthesis.** Gold nanorods (NRs) were prepared via a seed-mediated growth. First, CTAB-capped Au seeds were synthesized by chemical reduction of $HAuCl_4$ with $NaBH_4$: 7.5 ml CTAB (0.1M) aqueous solution was mixed with 100 μl $HAuCl_4$ (24 mM) and diluted with water to 9.4 ml. Then, 0.6 ml ice-cold $NaBH_4$ (0.01M) was added while stirring magnetically. After 3 min, the stirring was stopped and the seed solution was kept undisturbed at room temperature for 30 min prior to any further experiment. The seeds

can be used within 2-5 h after preparation. After that, the growth solution of the Au NRs was prepared, which consisted of 100 ml CTAB (0.1 M), 2.04 ml $HAuCl_4$ (0.024 M), 2 ml $H_2SO_4$ (0.5 M), 0.4 ml $AgNO_3$ (10 mM), and 800 μL AA (0.1 M). 240 μl seed solution was added to the above growth solution to initiate the growth of the Au NRs. After 12 h, the Au NRs were purified by centrifugation twice (12000 rpm for 5 min). The precipitates were collected and redispersed in deionized water. The volume is 100 ml.

**Characterization.** The UV-vis-NIR absorption spectra evolution during the aggregation before and after addition of peptides was obtained from Varian Cary 50 using a scanning kinetic mode.

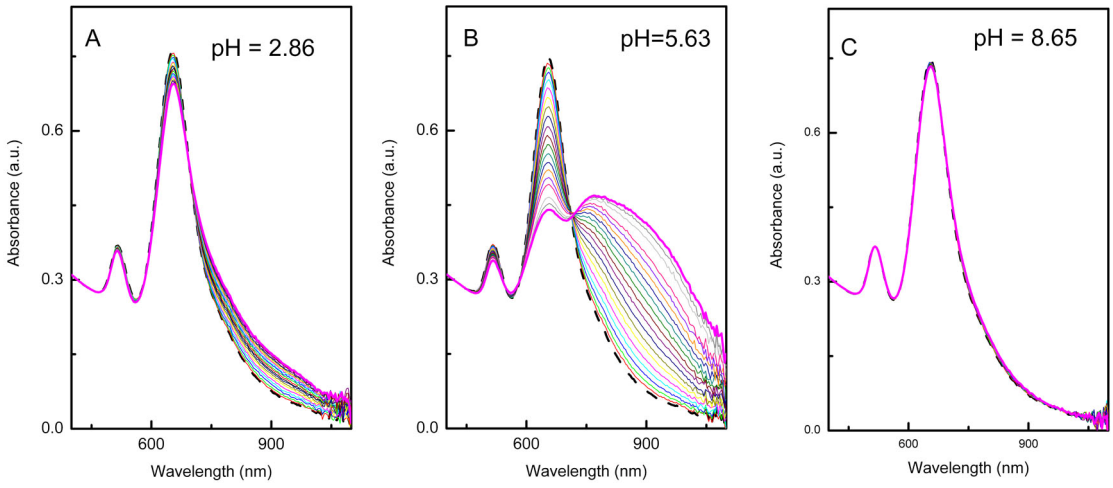
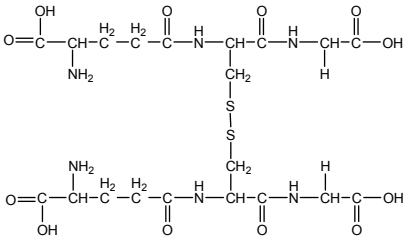
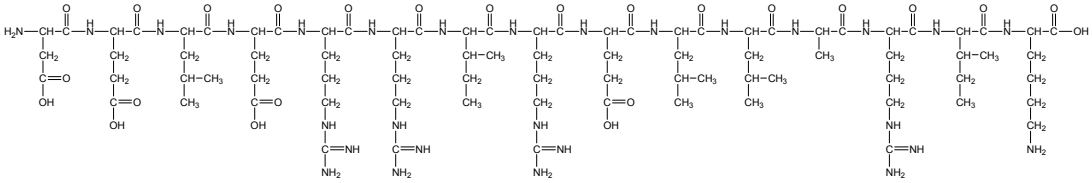


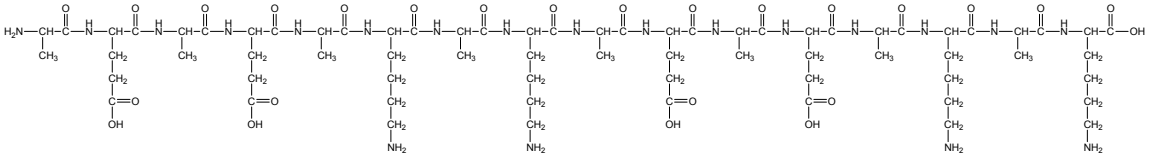

Fig. S1 4MP-induced Au NRs EE assembly via hydrogen bond between 4MP protonated and unprotonated states. (Conditions: CTAB=0.5 mM, NaCl=0.1 M, 4MP=6μM. Solution pH were adjusted by adding certain amount of 0.1M HCl or 0.01M NaOH.)



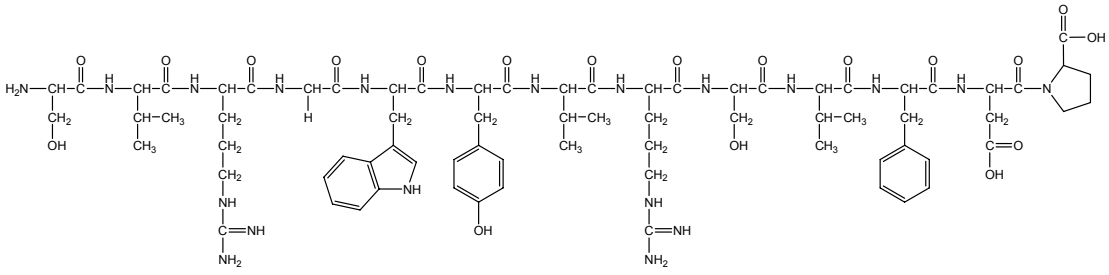
GS-SG



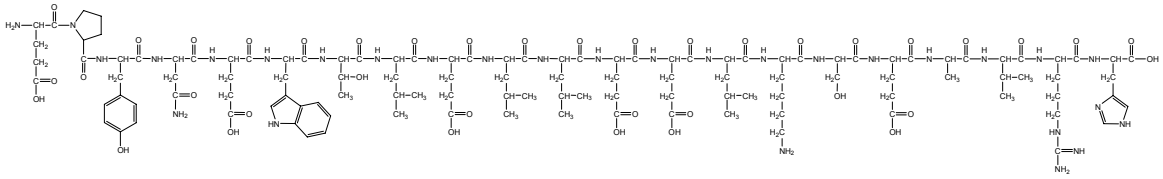
P15



P16



P13



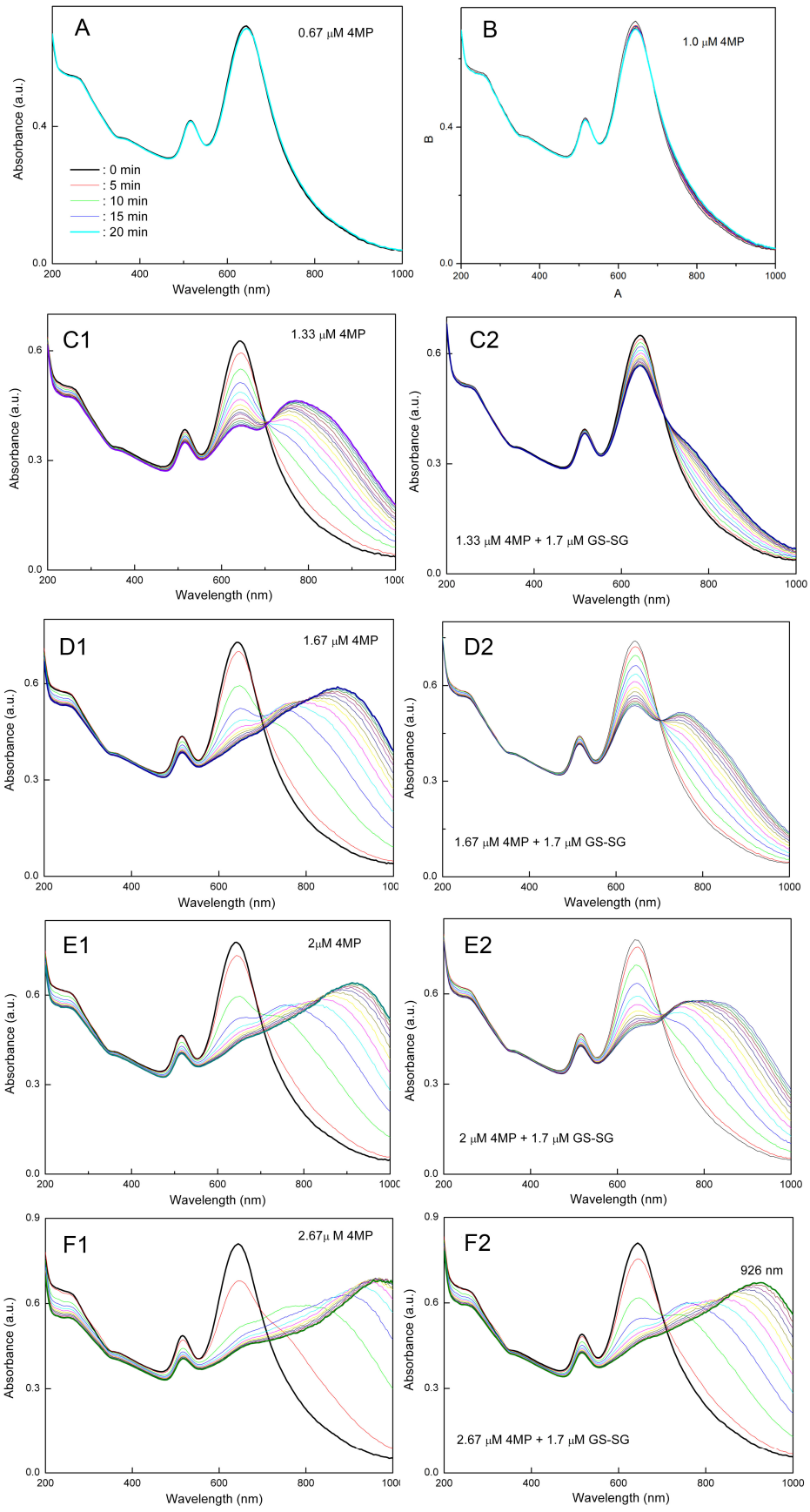
P21

Fig. S2 Peptide sequences of GS-SG, P15, P16, P13 and P21.

Table 1 Molecular weight (M. W.), isoelectric point (pI) and hydrophilicity of peptides

| Peptide | M. W. | pI | Hydrophilicity* |
|---|---|---|---|
| P15 | 1926.4 | 6.31 | 1.49 |
| P16 | 1615.8 | 6.33 | 1.25 |
| P13 | 1568.4 | 8.46 | -0.24 |
| P21 | 2586.1 | 4.47 | 0.41 |

* reference：T. P. Hopp, K. R. Woods, *Proc. Natl. Acad. Sci. USA*, 1981, **78**, 3824.


A
0.67 μM 4MP
: 0 min
: 5 min
: 10 min
: 15 min
: 20 min
Absorbance (a.u.)
Wavelength (nm)
B
1.0 μM 4MP
A
C1
1.33 μM 4MP
C2
1.33 μM 4MP + 1.7 μM GS-SG
D1
1.67 μM 4MP
D2
1.67 μM 4MP + 1.7 μM GS-SG
E1
2μM 4MP
E2
2 μM 4MP + 1.7 μM GS-SG
F1
2.67μ M 4MP
F2
926 nm
2.67 μM 4MP + 1.7 μM GS-SG

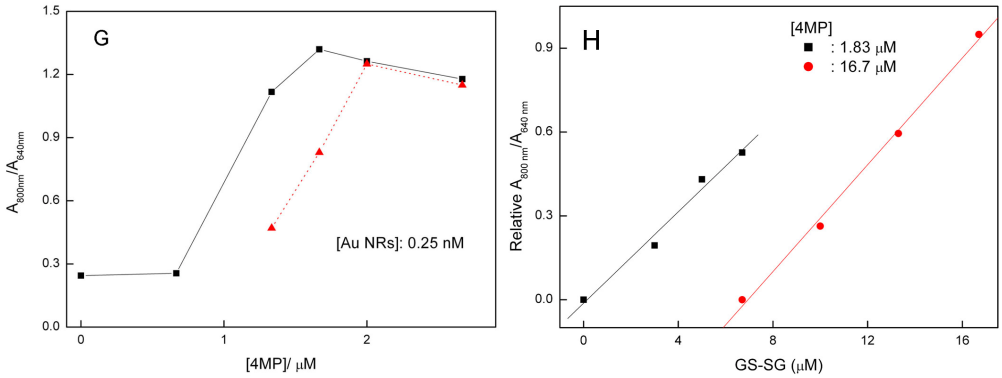



Fig. S3 Effects of 4MP (A, B, C1, D1, E1, and F1) and (4MP + GS-SG) (C2, D2, E2, and F2) on aggregating kinetics of Au NRs, optimization of 4MP/Au NRs ratio for detection of GS-SG (G), and variation of 4MP/Au NRs ratio can be used to change detection limit (H).

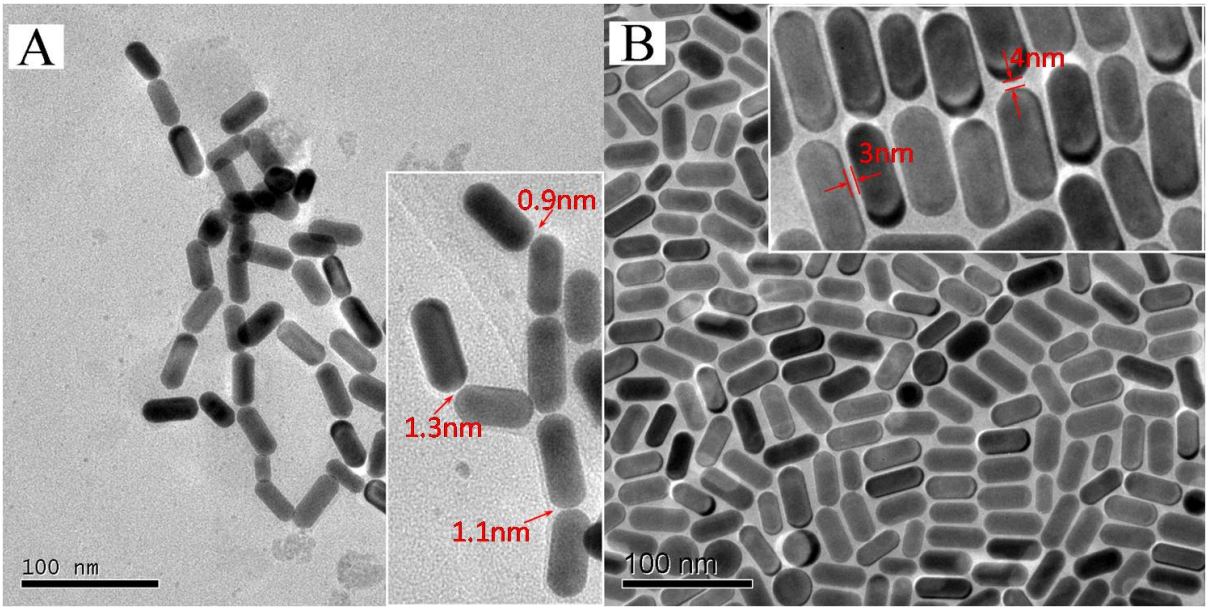



Fig. S4 TEM images of 4MP-induced Au NRs assemblies (A) and original Au NRs (B).

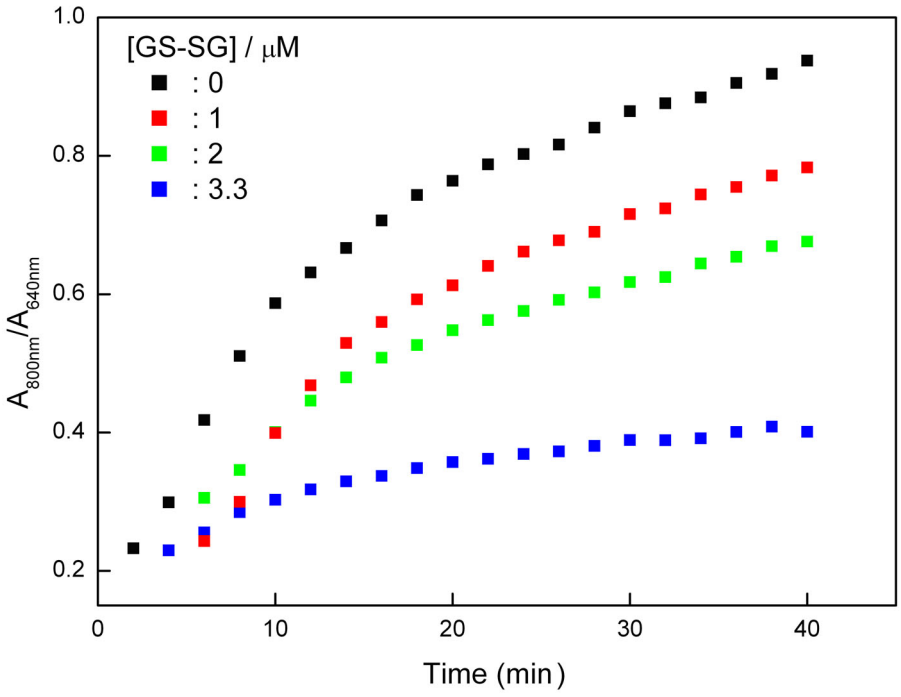



Fig. S5 Aggregating kinetics of Au NRs at different GS-SG concentrations. [4MP] is fixed at 1.33 μM.

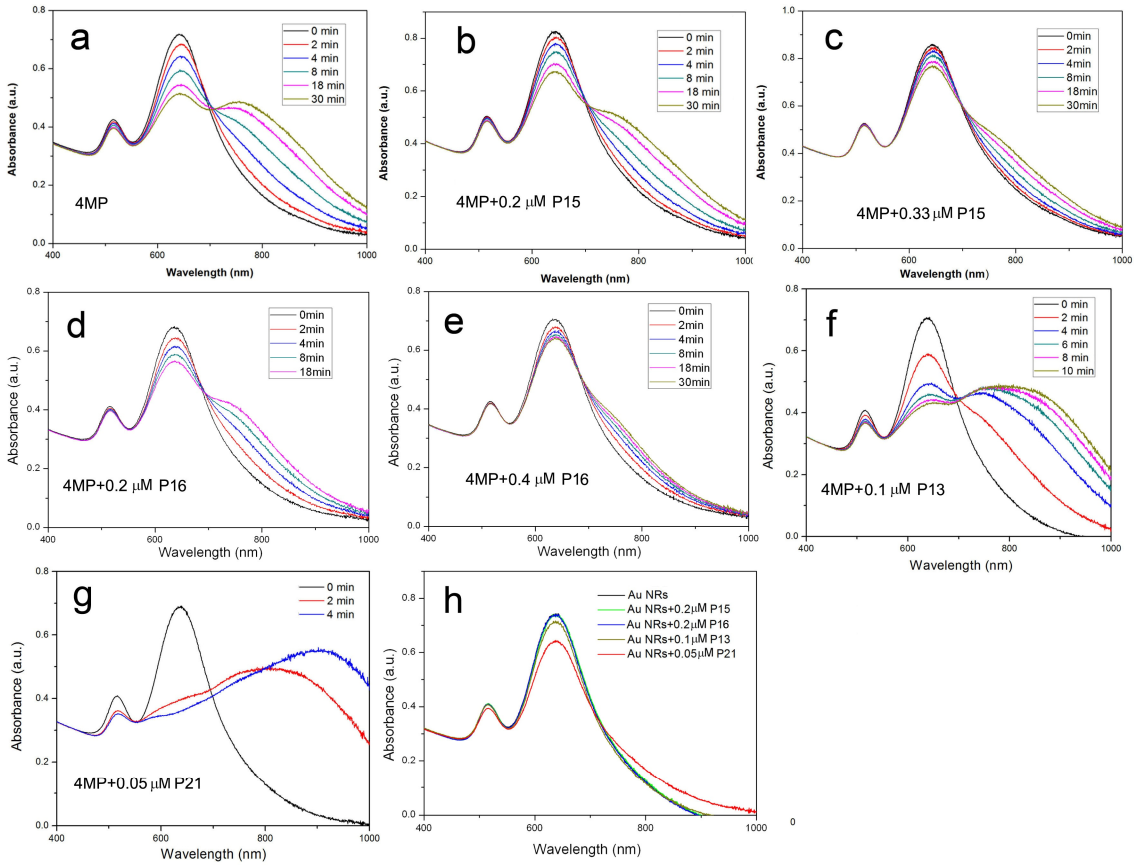



Fig. S6 Spectra evolution of Au NRs after addition of 1.33 μM 4MP (a) and the mixtures of 4MP and various peptides (b-g). The control spectra without 4MP are shown in h.

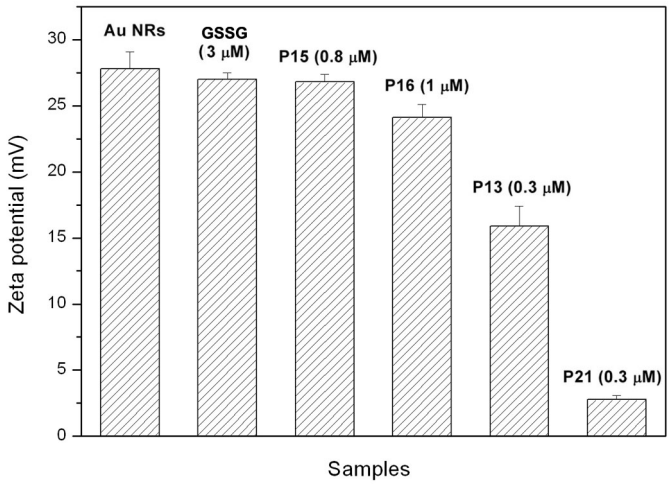



Fig. S7 Effects of peptides on the Zeta potentials of the Au NRs.

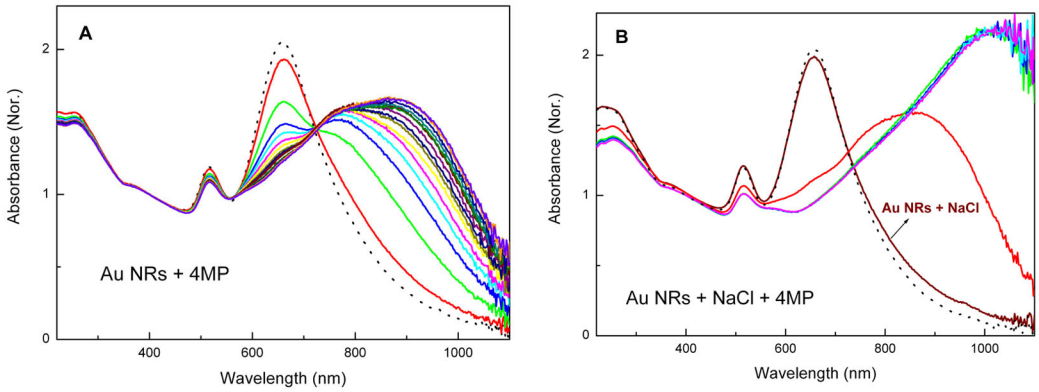



Fig. S8 Evolution of UV-vis-NIR absorption spectra of 4MP- Au NRs assemblies with an interval of 2 min: (A) without NaCl and (B) with 1mM NaCl. Addition of NaCl accelerates assembling kinetics and enhances aggregation degree. In contrast, without 4MP, 1mM NaCl only leads to a slight aggregation after 10 min.

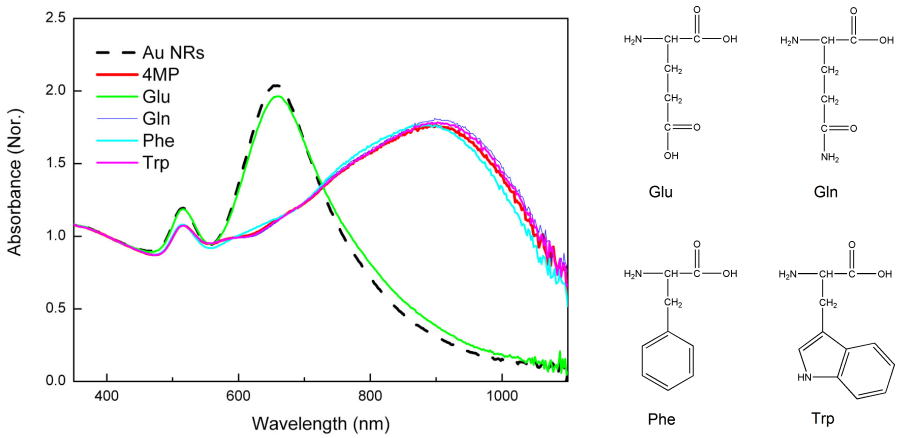



Fig. S9 Effects of several amino acids on the 4MP-induced Au NRs assembly after 30 min incubation. Condition: [4MP] = 4.5 μM, [Au NRs] = 0.25 nM, and [amino acid] = 50 μM. Amino acids with carboxylic groups exhibit inhibiting effect whereas other amino acids (either hydrophobic or hydrophilic) show no impact on assembly.