

Supplementary Information

Membrane-Targeting Mechanism of Host Defense Peptides Inspiring the Design of Polypeptide-Conjugated Gold Nanoparticles Exhibiting Effective Antibacterial Activity against Methicillin- Resistant *Staphylococcus aureus*

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Fig. S1 GPC traces of peptide polymer DLL₉₀BLG₁₀ at the sidechain protected stage using DMF as the mobile at a flow rate of 1 mL/min.

Fig. S2 ¹H NMR spectrum of peptide polymer DLL₉₀BLG₁₀ after deprotection (400 MHz, D₂O).

Fig. S3 TGA curves of Au NPs and Au@P NPs

Table S1 MIC and MBC values of Au@P NPs and free peptide polymers against Gram-positive bacteria.

Table S2 MIC and MBC values of Au@P NPs and free peptide polymers against Gram-negative bacteria.

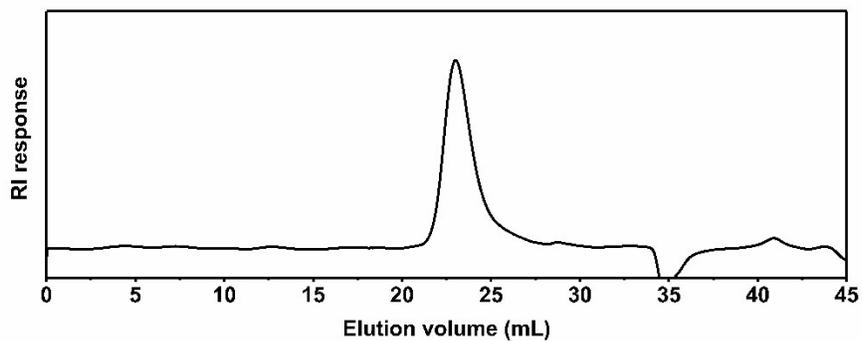


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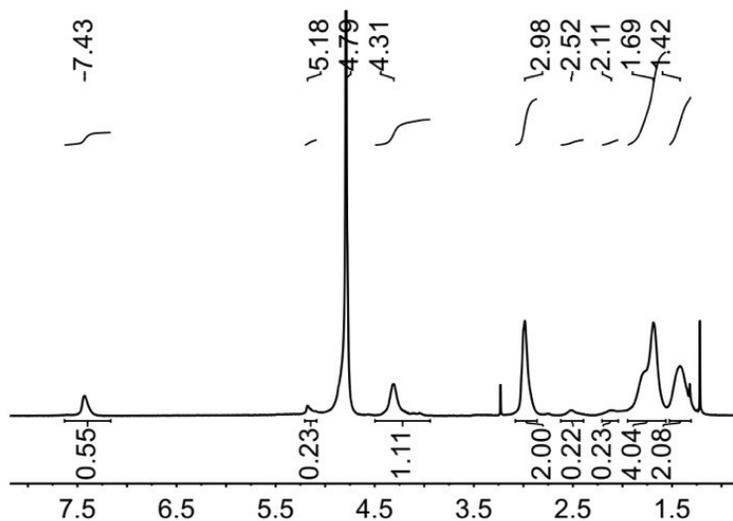


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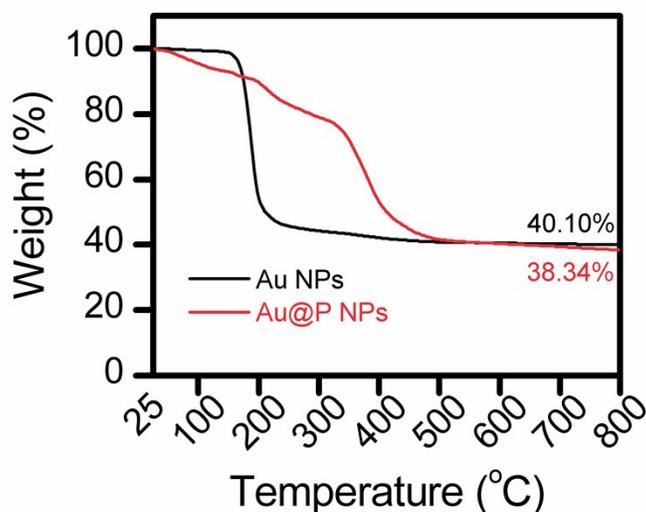


Fig. S3 TGA curves of Au NPs and Au@P NPs. The annotated number refers to the percentage of residual mass.

Calculation degree of peptide polymer conjugation to Au NPs from TGA results.¹ As shown in Equation S1, the weight of peptide polymer in Au@P nanoparticles was divided by the molecular weight of peptide polymer and multiplied by Avogadro's number to calculate the number of peptide polymer molecules lost. The weight of one Au nanoparticle was calculated from its volume (one Au nanoparticle's diameter is 12 nm) and density (19.32 g/cm³), and result is around 1.748×10^{-17} g/NP. Then the rest weight of Au@P nanoparticles was divided by the weight of one Au nanoparticle to calculate the number of Au nanoparticles. Finally, the number of peptide polymer molecules lost was divided by the number of Au nanoparticles to obtain the average number of peptide polymer chains per Au nanoparticle. The result is about 31 chains per Au NP.

$$N_{\text{graftes per Au NP}} = \frac{\left(\frac{W_{\text{peptide polymer in Au@P nanoparticles}}}{M_{\text{peptide polymer}}} \right) \times N_A}{\frac{W_{\text{rest weight of Au@P nanoparticles}}}{W_{\text{one Au nanoparticle}}}} \quad (\text{Equation S1})$$

(N represents chain number, W represents weight, M represents molecular weight and N_A represents Avogadro's number)

Table S1 MIC and MBC values of Au@P NPs and free peptide polymers against Gram-positive bacteria.

strains	Au@P NPs		DLL ₉₀ BLG ₁₀	
	MIC (µg/mL)	MBC (µg/mL)	MIC (µg/mL)	MBC (µg/mL)
<i>S. aureus</i> USA300 LAC	6.25	12.5	6.25	12.5
<i>S. aureus</i> 2904	12.5	12.5	12.5	12.5
<i>S. aureus</i> 2902	12.5	12.5	6.25	12.5
<i>S. aureus</i> 2802	12.5	12.5	12.5	12.5
<i>S. aureus</i> 2202	12.5	12.5	12.5	12.5
<i>S. aureus</i> ATCC6538	12.5	25	12.5	12.5
<i>S. haemolyticus</i> 1303	3.13	3.13	3.13	3.13
<i>B. subtilis</i> BR151	3.13	3.13	3.13	3.13

Table S2 MIC and MBC values of Au@P NPs and free peptide polymers against Gram-negative bacteria.

strains	Au@P NPs		DLL ₉₀ BLG ₁₀	
	MIC (µg/mL)	MBC (µg/mL)	MIC (µg/mL)	MBC (µg/mL)
<i>E. coli</i> ATCC25922	>200	>200	>200	>200
<i>E. coli</i> 1608	>200	>200	>200	>200
<i>A. b.</i> BAA-747	>200	>200	>200	>200
<i>K. p.</i> ATCC700603	>200	>200	>200	>200

Reference

1. L. Pu, J. Xu, Y. Sun, Z. Fang, M. B. Chan-Park and H. Duan, *Biomater Sci*, 2016, **4**, 871-879.