

Supplementary Information

Engineering hydrophobic and electrostatic interactions for selective inactivation of bacteriophages by mixed-ligand nanoparticles

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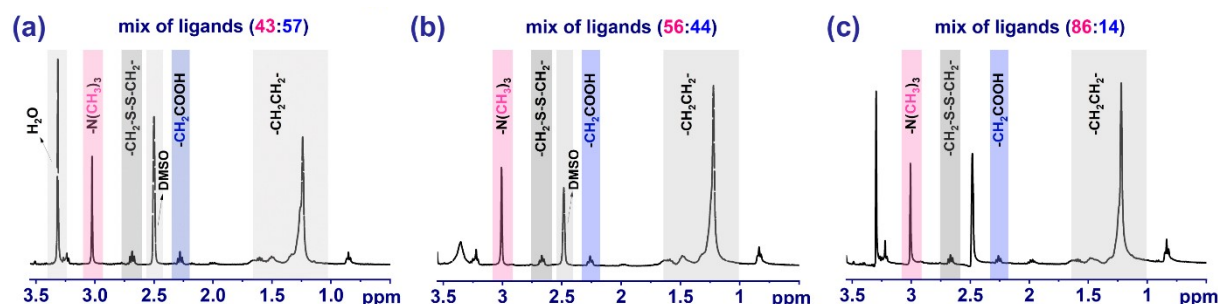


Figure S1: Proton NMR spectrum of the MLNPs composed of (a) 43% TMA and 57% MUA, (b) 56% TMA and 44% MUA, and (c) 86% TMA and 14% MUA.

Table S1: Chemical shifts of relevant H groups (s – singlet; t – triplet; q – quartet; m – multiplet)

Type of H Group	Chemical Shift (ppm)
<u>-CH₂</u> -N ⁺ (CH ₃) ₃	3.29 – 3.21 (m)
-CH ₂ -N ⁺ (<u>CH₃</u>) ₃	3.02 (s)
<u>-CH₂</u> -SS- <u>CH₂</u> -	2.72 – 2.65 (t)
<u>-CH₂</u> -COOH	2.30 – 2.23 (t)
<u>-CH₂</u> -COO ⁻	2.20 – 2.15 (t)
CH ₂ - <u>CH₂</u> -CH ₂	1.71 – 1.19 (m)
-CH ₂ - <u>CH₃</u>	0.88 – 0.80 (t)
<u>-CH₂</u> -SH	2.56 – 2.48 (q)
-CH ₂ - <u>SH</u>	2.22 – 2.17 (t)

Figure S2 presents the TGA curves of nanoparticles functionalized with TMA (100%), MUA (100%), and mixed-ligand nanoparticles functionalized with TMA:MUA:DDT. As shown, Au@TMA and Au@MUA nanoparticles exhibit residual masses of 80.05 wt% and 79.15 wt% at 500 °C, respectively, with the observed mass losses attributed to the thermal degradation of TMA and MUA ligands on the nanoparticle surfaces. Moreover, mixed-ligand nanoparticles functionalized with TMA:MUA:DDT exhibit a total mass loss of 20.85 wt%, which corresponds to the degradation of TMA, MUA, and DDT ligands on the surfaces of the mixed-ligand Au nanoparticles.

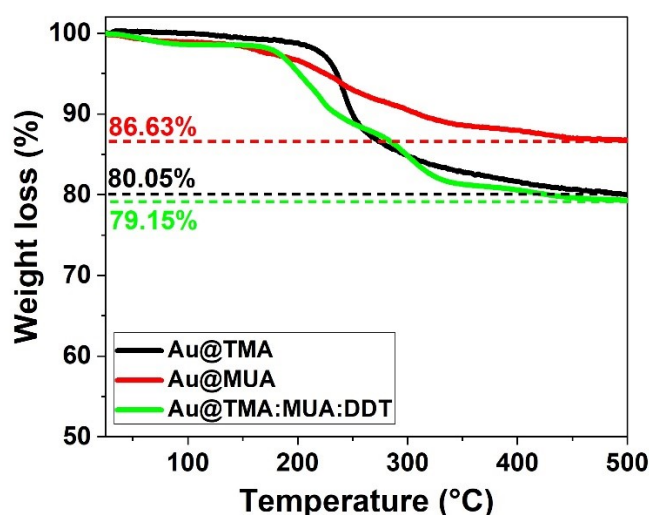


Figure S2: Thermogravimetric analysis of Au@TMA, Au@MUA, and Au@TMA:MUA:DDT.

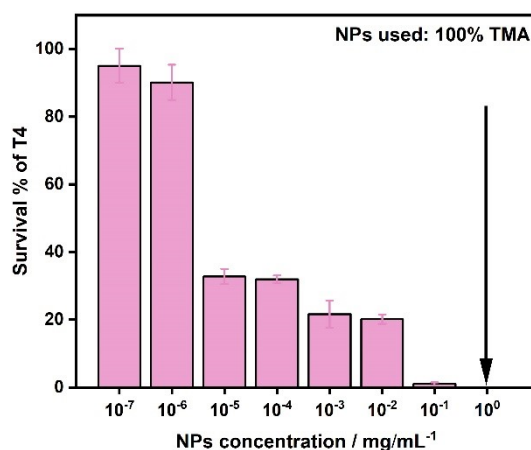


Figure S3: Dosage compensation of the survival % of T4 bacteriophages against 100% positive (only TMA, 100:0:0) nanoparticles. The virions were exposed to MLNPs concentrations, ranging from 10^{-7} mg/mL to 1 mg/mL. The starting concentration of T4 was 10^7 PFU/mL.