Peptide-Gold Nanoparticle Conjugates as Artificial Carbonic Anhydrase Mimics

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Supporting Information

Experimental Section

FT-IR Spectroscopy

IR-spectra were recorded using an ATR-FT/IR-4100 by Jasco, averaging 100 scans with 2 cm^{-1} resolution. Lyophilized peptide and peptide-gold nanoparticle conjugates were placed on the diamond crystal. IR spectra were recorded, taking into account the corresponding background.

Transmission Electron Microscopy (TEM)

Aliquots (5 µL) of the aqueous peptide or Pep-Au-NP samples were applied to a Formvar/carbon covered copper grid (400 mesh, PLANO GmbH, Wetzlar) which was hydrophilized by glow discharging at 8 W in a BALTEC MED 020 device for 60 s directly before use. After 60 s of Au-NP sedimentation excess liquid was removed with filter paper and the grid was air-dried for at least 18 h. The grid was then transferred to a Talos L120C transmission electron microscope (FEI Company, Oregon) equipped with a LaB_6 electrode operating at an acceleration voltage of 120 kV. Image data were recorded using a 4k × 4k Ceta CMOS camera and nanoparticle size and size

distribution was determined using ImageJ (Image processing and analysis in JAVA) V 1.50 [1] by analyzing at least 500 particles.

Calculation of gold nanoparticle concentration

Concentration of Au-NP dispersion after the reaction was calculated according to equations reported by Liu *et al.* [2]. Briefly, the average number of gold atoms per nanoparticle (N) was calculated using Eq. (1), which assumes spherical shaped particles and a uniform fcc structure by taking into account the density of fcc gold (ρ = 19.3 g/cm^3) and the atomic weight of gold (M_{Au} = 197 g/mol). Average diameter D was determined by TEM.

$$N = \frac{\pi \rho D^3}{6M} = 30.89602 D^3 \qquad (1)$$

The molar concentration of the gold nanoparticle dispersion was calculated by dividing the overall amount of gold salt added to the reaction solution (which corresponds to the total number of gold atoms N_{total}) by the average number of gold atoms per gold nanoparticle (N) according to Eq. (2), where V is the total reaction volume and N_A is the Avogadro constant.

$$\mathrm{C} = \frac{\mathrm{N_{total}}}{\mathrm{NVN_A}} \qquad (2)$$

Supporting Figures

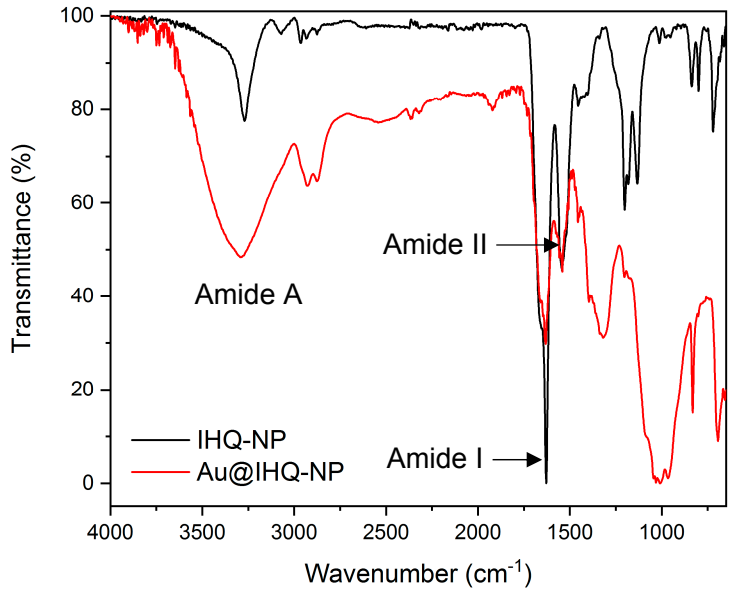

Figure S1. Normalized FT-IR spectra of IHQ-NP and Au@IHQ-NP showing the successful conjugation of IHQ-NP to the gold nanoparticles.

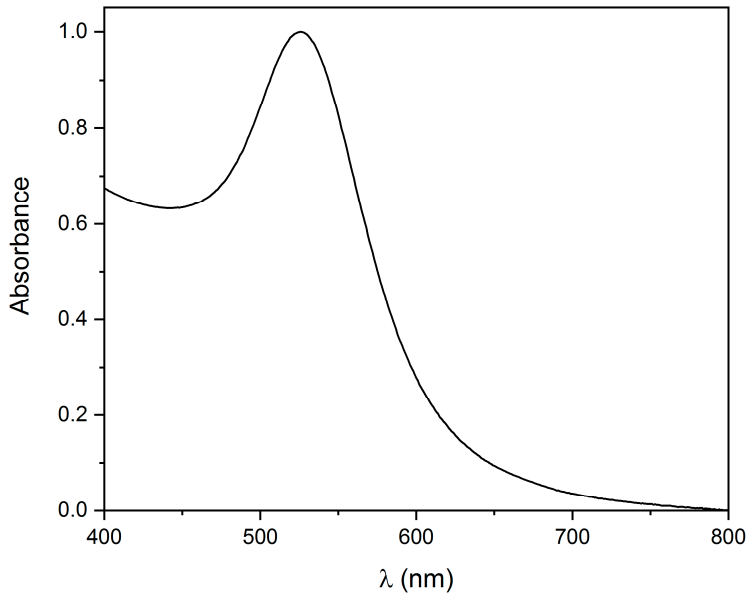

Figure S2. Normalized UV/Vis-Spectra of Au@IHQ-NP showing the surface plasmon resonance absorption maximum at 525 nm.

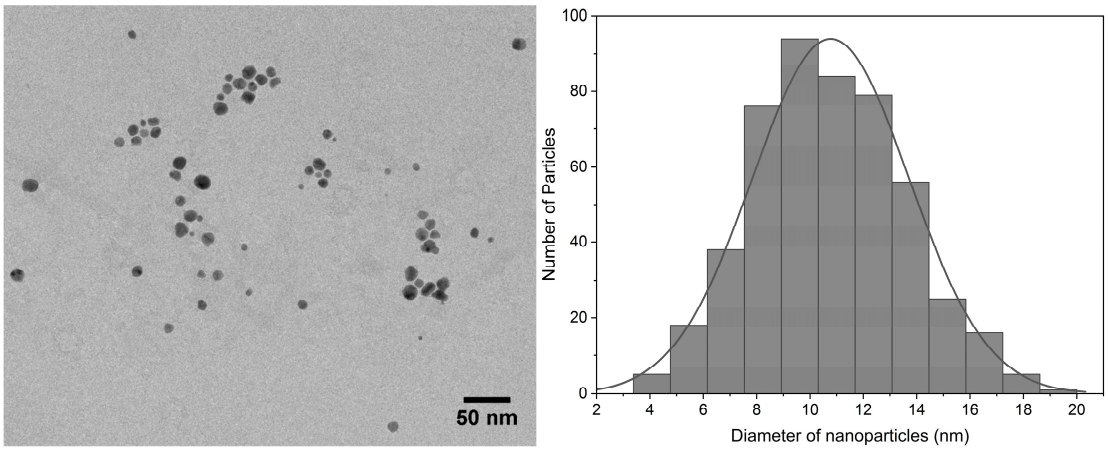

Figure S3. (left) TEM characterization of Au@IHQ-NP showing spherical gold nanoparticles with a mean diameter of 10.8 ± 2.8 nm and (right) the corresponding histogram. Scale bar corresponds to 50 nm.

References

1. Schneider, C. A.; Rasband, W. S.; Eliceiri, K. W. NIH Image to ImageJ: 25 Years of Image Analysis. *Nat. Methods* **2012**, *9* (7), 671–675. https://doi.org/10.1038/nmeth.2089.

2. Liu, X.; Atwater, M.; Wang, J.; Huo, Q. Extinction Coefficient of Gold Nanoparticles with Different Sizes and Different Capping Ligands. *Colloids Surfaces B Biointerfaces* **2007**, *58* (1), 3–7. https://doi.org/10.1016/j.colsurfb.2006.08.005.