Electronic Supplementary Material (ESI) for Biomaterials Science.

Supporting Information

Effects of Aspect Ratio of Plasmonic Gold Nanorods on the Inhibition of Lysozyme Amyloid Formation

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# Equally contributed

Determination of gold nanorod concentrations:

The detailed calculations on the concentrations of GNRs is provided below and also in the supporting information of the revised manuscript. The concentration of gold nanorods has been calculated by following the literature reported procedure for the spherical gold nanoparticles[1]. We have adopted the same procedure to determine the concentration of rod shaped gold nanoparticles (GNRs) by assuming them as cylinders. For example, detailed calculations were provided for a representative GNR of AR 2.2.

Step-1: To determine the average number of gold atoms per nanorod.

Assuming a cylindrical shape and a uniform face-centered cubic structure[2], the average number of gold atoms (*N*) per nanorod was calculated by Eq. (1), where *ρ* is the density for fcc gold (19.3 g/cm^3)[3], *D* is the diameter, l is the length of GNRs and *M* stands for atomic weight of gold (197 g/mol).

N = (π D2lρ/2)*M …….(1)

= 3.14 × 19.647 × 19.647 × 29.833/2 × 197 = 1771.25

Step-2: To determine the molar concentrations of GNRs.

The molar concentration (*C*) of the GNRs were calculated by dividing the total number of gold atoms (N_{total}, equivalent to the initial amount of gold salt added to the reaction solution) over the average number of gold atoms per nanorod (N) according to Eq. (2), where V is the volume of the reaction solution in liter and N_A is the Avogadro's constant. We assume that the reduction of gold was 100%.

$C = N_{total}/N_A VN$…….(2)

During the synthesis of GNRs, the concentration of gold used was 1 mM, in a reaction volume of 50 mL. The mass of gold used (W) is 20 mg.

If 393.83 g of gold correspond to N_A of atoms, then 20 mg of gold should correspond to $N_A \times 5 \times 10^{-4}$ atoms (Eq. (3))

$N_{total} = N_A \times 5 \times 10^{-4}$…….(3)

Now substitute Eq. (3) in (2)

Then, the concentration of GNRs with AR 2.2 is 4.2 nM. In a similar manner, we have determined the concentrations of GNRs with AR 3.1 is 4.4 nM, and for AR 4.2 is 5.0 nM respectively.

Molecules used for amyloid inhibition	Size	Target protein	Reference
Au NPs	30 nm	Aβ	4
Au NPs & Au NRs	30 nm & 83 nm	Lysozyme	(Reference no. 25 in main text)
Au NRs	15-50 nm	Aβ	(Reference no. 44 in main text)
CMdex NPs	207 nm	Lysozyme	5
Carbon dots	< 6 nm	Insulin	6
Histidine based polymer coated NPs	5-100 nm	Aβ	7

Table S1: Comparison of different modalities to inhibit amyloids (NPs represents nanoparticles).

Entry	Mean length of the nanorod (L, nm)	Mean diameter of the nanorod (D, nm)	Aspect ratio (AR, L/D)	Transverse surface plasmon resonance (TSPR)	Longitudinal surface plasmon resonance (LSPR)
GNR1	46.9 ± 3.7 nm	21 ± 2.3 nm	2.2	514 nm	643 nm
GNR2	52.5 ± 1.56 nm	16.9 ± 1.6 nm	3.1	512 nm	707 nm
GNR3	51.2 ± 4.8 nm	12.1 ± 1.3 nm	4.2	510 nm	802 nm

Table S2: Physico-chemical characteristics of GNRs.

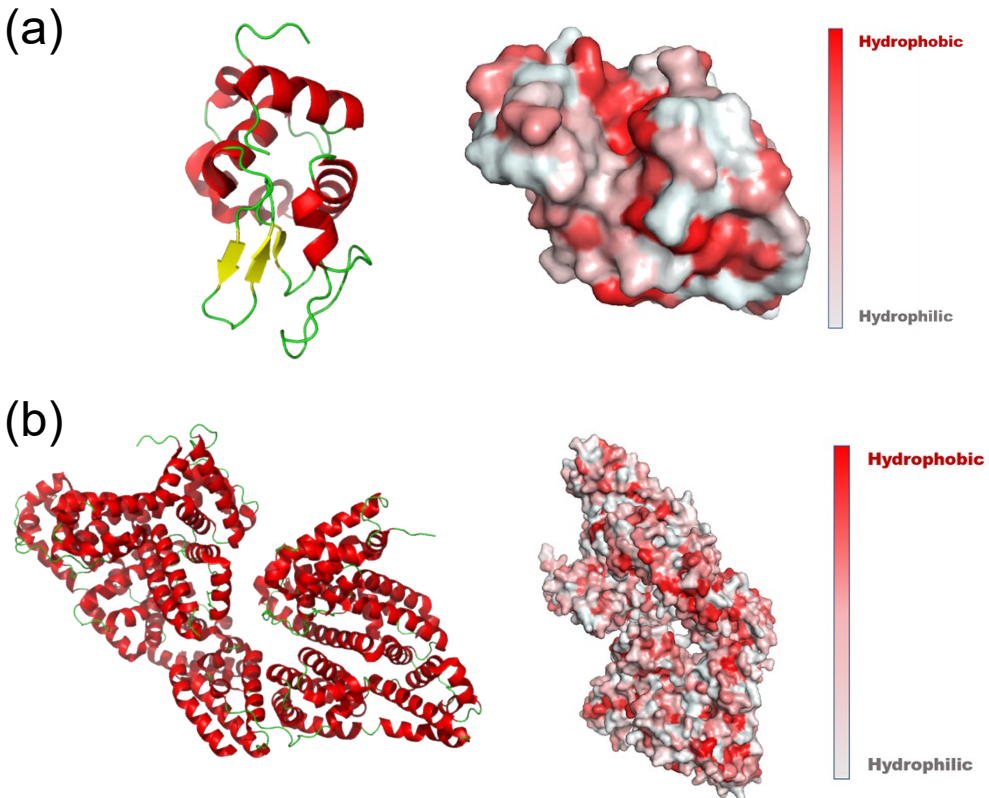

Figure S1: Representation of crystal structures comprising α-helices (red), β-sheet (yellow) and random coil (green) and surface hydrophobicity. (a) Hen Egg White lysozyme (HEWL; PDB ID: 1GWD) and (b) Bovine Serum Albumin (BSA; PDB ID: 4F5S). The structures were drawn using PyMOL (Schrödinger Inc., LLC, New York).

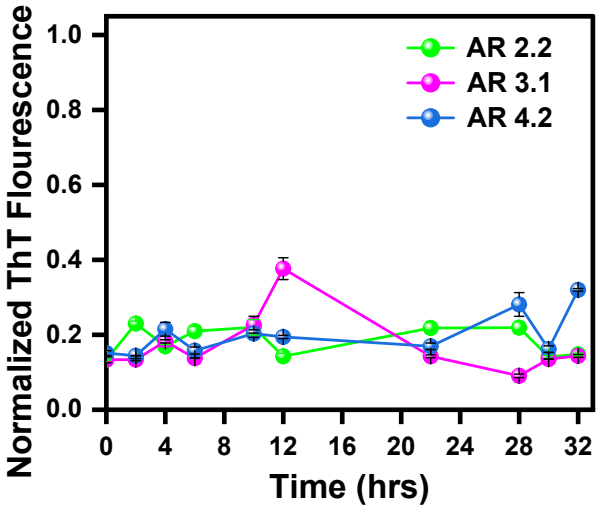

Figure S2: ThT fluorescence for GNRs recorded over time under the same aggregation conditions.

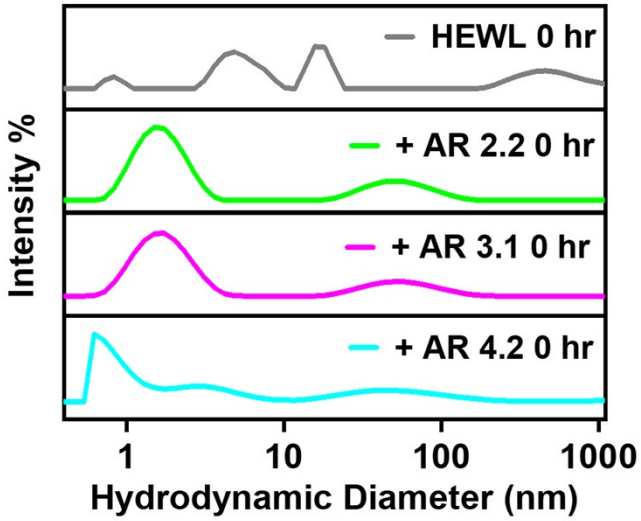

Figure S3: Dynamic light scattering data for HEWL alone and with all three AR GNRs (AR 2.2, AR 3.1 and AR 4.2) at the 0 hour (initial stage).

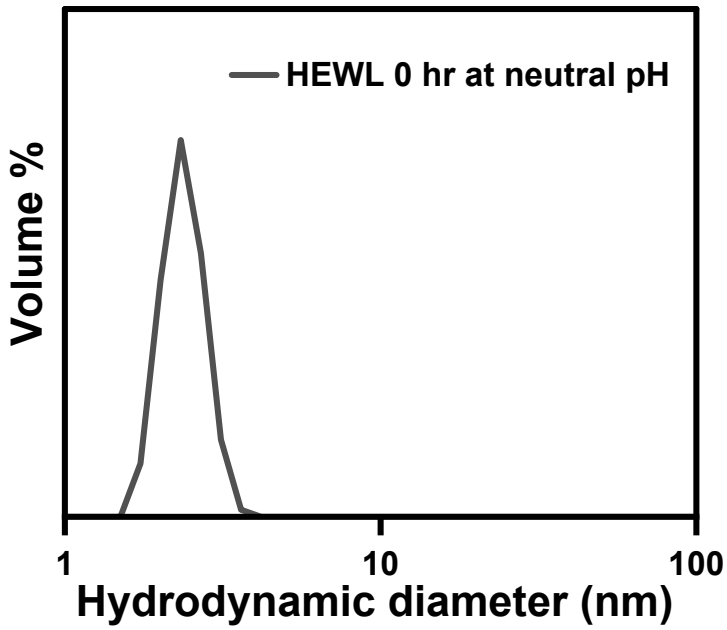

Figure S4: Measurement of hydrodynamic diameter of HEWL at neutral pH.

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