The originally published ESI document for DOI: 10.1039/c7me00091j was replaced with this version on 13th January 2020

Electronic Supplementary Information

Identifying Peptide Sequences that Can Control the Assembly of Gold Nanostructures

Hye-Eun Lee[1†], Jaehun Lee[1†], Misong Ju[1], Hyo-Yong Ahn[1], Yoon Young Lee[1], Hyung-Seok Jang[2] and Ki Tae Nam[1]*

[1]Department of Materials Science and Engineering
College of Engineering
Seoul National University
Gwanak-ro 1, Gwanak-Gu, Seoul 08826 (Korea)

[2]School of Chemical and Biological Engineering
College of Engineering
Seoul National University
Gwanak-ro 1, Gwanak-Gu, Seoul 08826 (Korea)

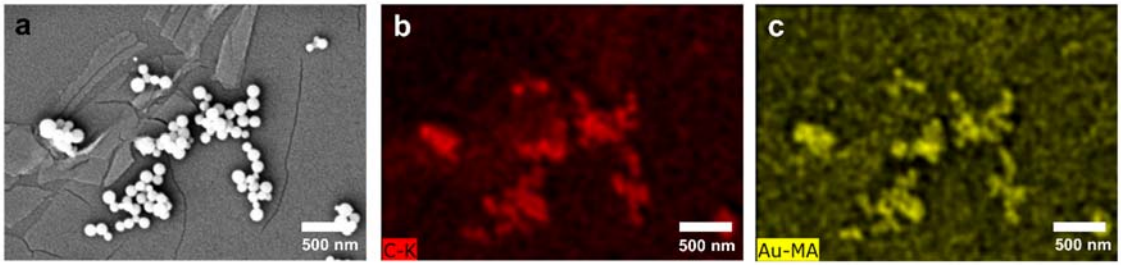

Fig. S1 SEM/EDS mapping images of gold nanoparticles and peptide hybrid film. (a) SEM image of the peptide sheets decorated with gold nanoparticles. (b, c) EDS mapping images show the elemental distributions of carbon (b) and gold (c).

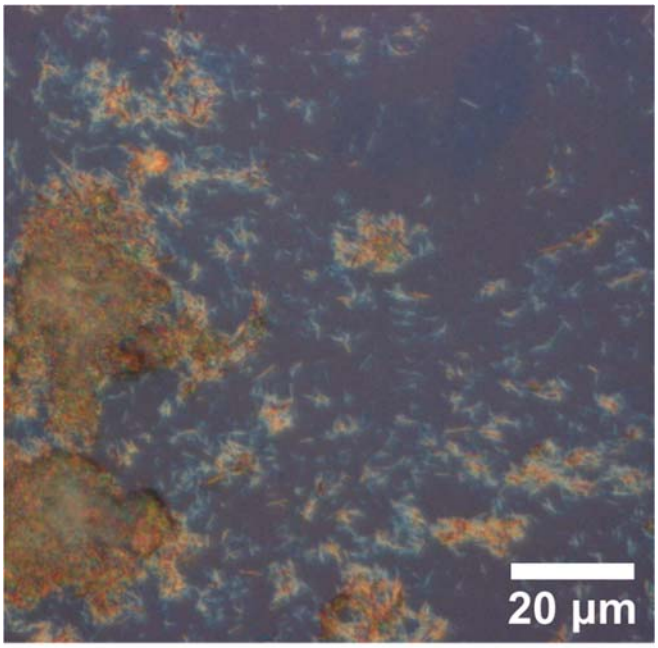

Fig. S2 Optical image of fibrillar aggregations. The sample was prepared by directly stamping from the water droplet when the concentration of gold was lower than 1 mM.

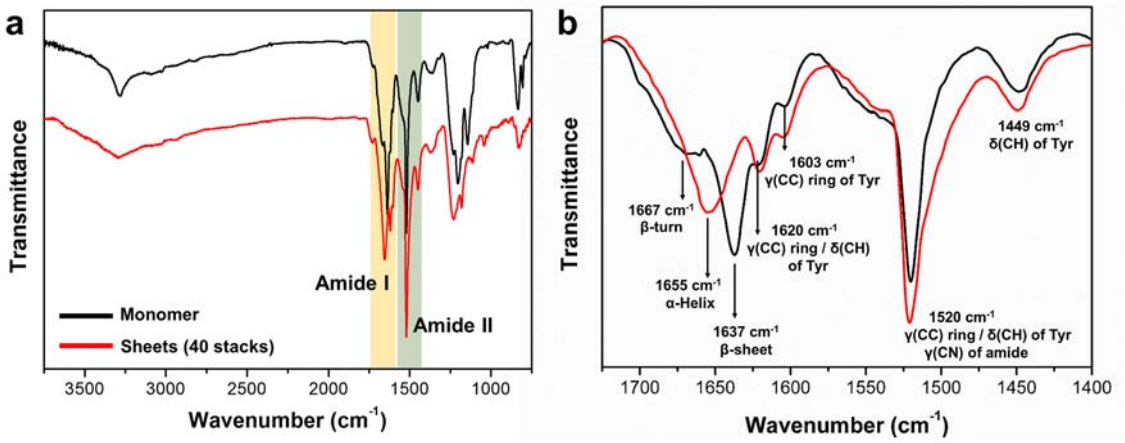

Fig. S3 FT-IR spectra of monomer peptide (black line) and film (red line). (a) Representative FT-IR spectrum of monomer YYCYY and stacked nanosheets in region of 3750 to 750 cm^{-1}. Vibrational bands of the amide I and amide II regions are indicated with vertical bars. (b) FT-IR spectra in amide I and II regions, highlighted in (a). γ and δ denote stretching vibration and in-plane bending vibration respectively.

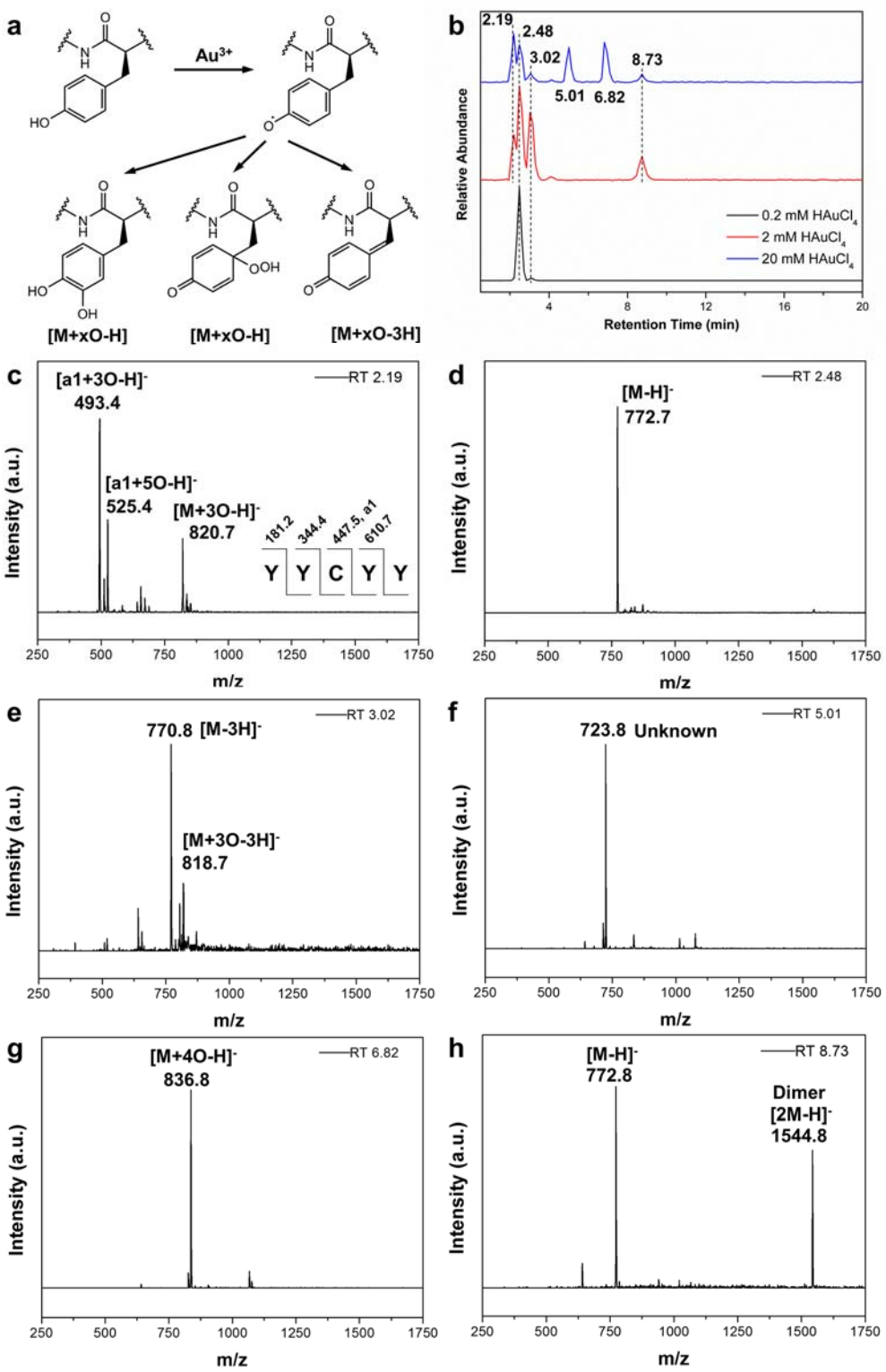

Fig. S4 Presence of oxidized tyrosines and dimer YYCYY analyzed by LC/MS. (a) Proposed oxidation pathways of tyrosine in this system. x denotes the number of added oxygen. (b) LC results of reaction products of YYCYY (1.5 mM) and $HAuCl_4$ (0.2, 2, 20 mM). (c-h) Electronspray Ionization MS data of each peak in LC spectrum.

Figure S4 shows LC/MS results obtained from the reaction of YYCYY peptide with $HAuCl_4$. In particular, there are four peaks in LC spectra when the added amount of $HAuCl_4$ was 2 mM where the concentration of facet formation occurs. The highest peak at retention time of 2.48 min corresponds to the unreacted monomer YYCYY, $[M-H]^-$, species (m/z 772.7). There was new significant peak came up at retention time of 8.73 min and the m/z 1544.8 of this peak can be assigned to the mass of the dimer YYCYY. Other m/z values of reaction products were matched with the suggested oxidized forms of tyrosine in Fig. S4a. In nature, tyrosine is involved in many protein oxidation processes, being one of the most easily oxidized amino acids. It is reported that tyrosine oxidation can occur through several routes, where the dominant pathway brings to the formation of 3,4-dihydroxyphenlalanine.[2] Besides tyrosine radical can undergo a number of oxidative post-translational modification to form hydroxyl-tyrosine, nitro-tyrosine, crosslinked-tyrosine, and halogenated tyrosine.[3] Such oxidation of tyrosine and nature of the oxidation products depend on the pH, nature of oxidizing agent and the condition of the reaction mixtures. The results clearly showed that tyrosine had a role to reduce gold cation for the formation of gold nanoparticles and tyrosine was oxidized into several forms.

Reference

[1] J. A. Stubbe and W. A. Van Der Donk, *Chem. Rev.*, 1998, **98**, 705–762.

[2] C. Houée-Lévin, K. Bobrowski, L. Horakova, B. Karademir, C. Schöneich, M. J. Davies and C. M. Spickett, *Free Radic. Res.*, 2015, **49**, 347–373.

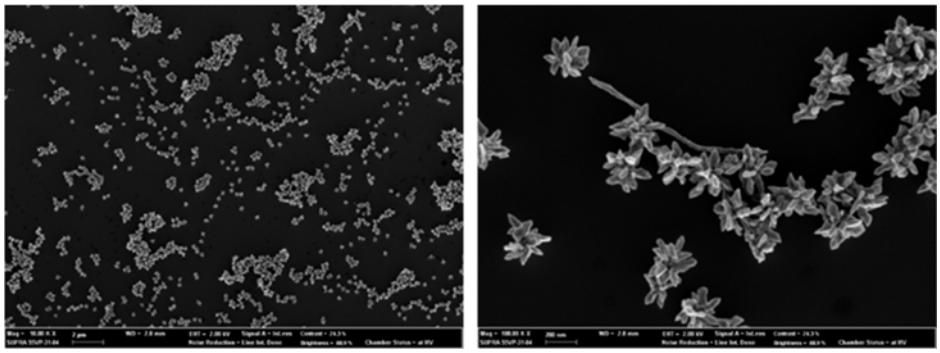

Fig. S5 Low magnification SEM images of petal like structure synthesized by L-GSH.

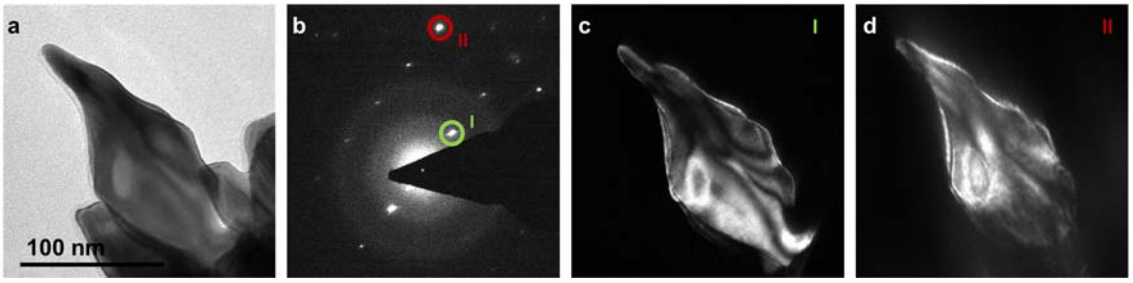

Fig. S6 TEM images and selected-area electron diffraction pattern of petal nanoparticle. (a) Bright field TEM image and (b) selected area electron diffraction pattern of petal structure. (c,d) Dark field images showing selected lattice orientation. Different aperture locations shown in colored circle in (b).

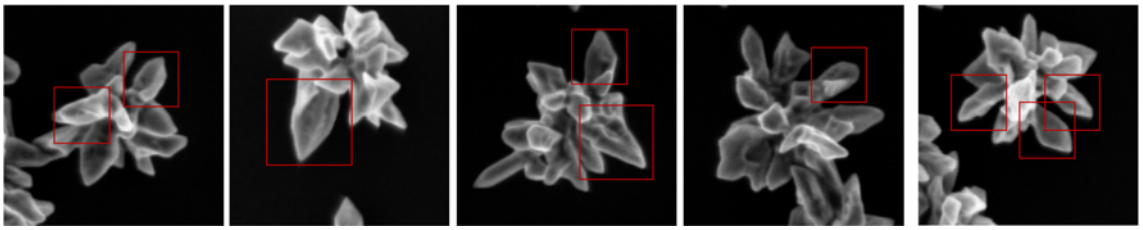

Fig. S7 SEM images of individual outspread petal nanoparticles prepared under L-GSH. Red box indicates partial structure shown in Fig. 4c

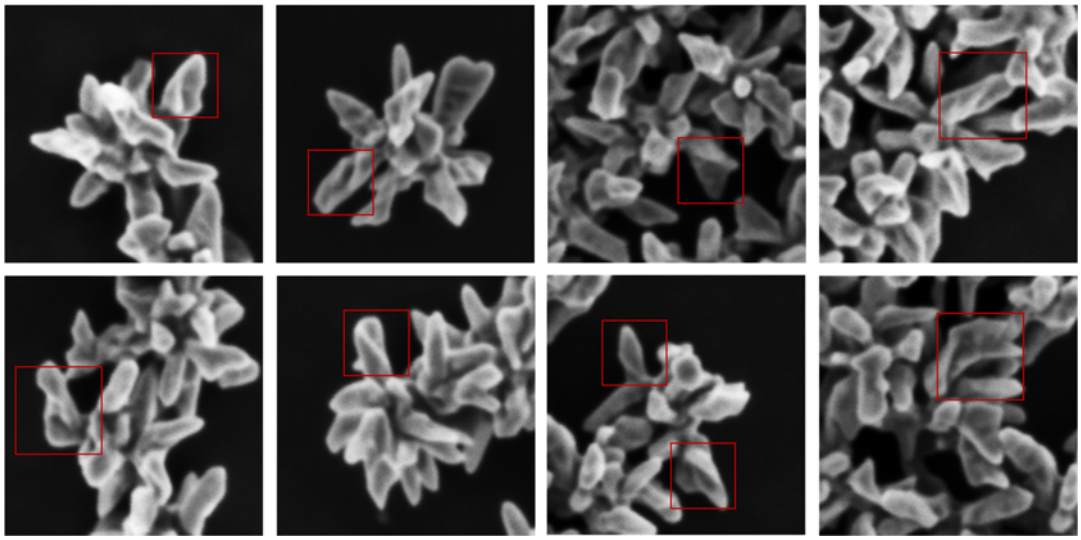

Fig. S8 SEM images of individual outspread petal nanoparticles prepared under D-GSH. Red box indicates partial structure shown in Fig. 4c

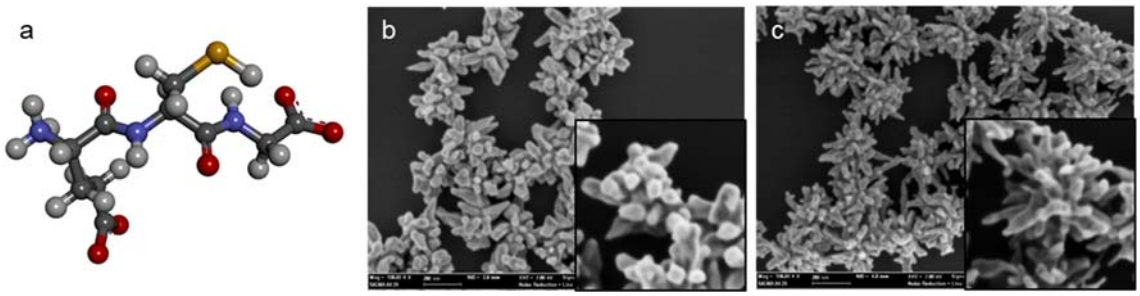

Fig. S9 Effect of isoglutathione (α-glutamylcysteinylglycine, ECG) on morphology. (a) Structure of ECG. SEM images of resultant nanoparticle synthesized under ECG with different concentration (b) 10 μM and (c) 20 μM of ECG.