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Biocompatible and Multifunctional Gold Nanorods for Effective Photothermal Therapy of Oral Squamous Cell Carcinoma

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Calculation

Assumption:

The diameter of GNRs is 11.1 nm and the length of GNRs is 48.3 nm. The length of a gold atom is 144 pm the area of a gold atom is 2.0736E-20 m^2. The density of gold is 19.3 g/cm^3. Totally 1E-8 mol of GNRs are coated with X mg of alginate.

Calculation:

The volume of a GNR is $(11.1E-9)^2$ x 3.14 x 48.3E-9 = 1.8686 E-23 m^3 and the surface area of a GNR is 11.1E-9 x 3.14 x 48.3E-9 + $(11.1E-9)^2$ x 3.14 / 4= 1.876E-15 m^2.

The weight of a GNR is 1.8686 E-23 x 1.93E7 = 3.606E-16 g

The number of GNR in a batch is 195E-8 / 3.606E-16 = 5.407E9 rod in a batch

The number of gold atom on the surface of a GNR is 1.876E-15 / 2.0736E-20 = 9.050E4 atoms and total number is 9.050E4 x 5.407E9 = 4.893E14 atoms = 8.128E-10 mol

Table S1 Quantification of thiol on cysteine modified alginate.

Alginate (mol)[#]	Cysteine (mol)	EDC (mol)	Thiol bond (μmol/g Alg)
1	0.5	10	143.7±15.0
1	1	10	268.8±12.2
1	1.5	10	280.4±24.3
1	1	-	12.9±0.64

[#]: Molecular weight used here is the weight of an alginate unit (β-D-mannuronate or a α-L-guluronate). One mole of alginate is 176 g.

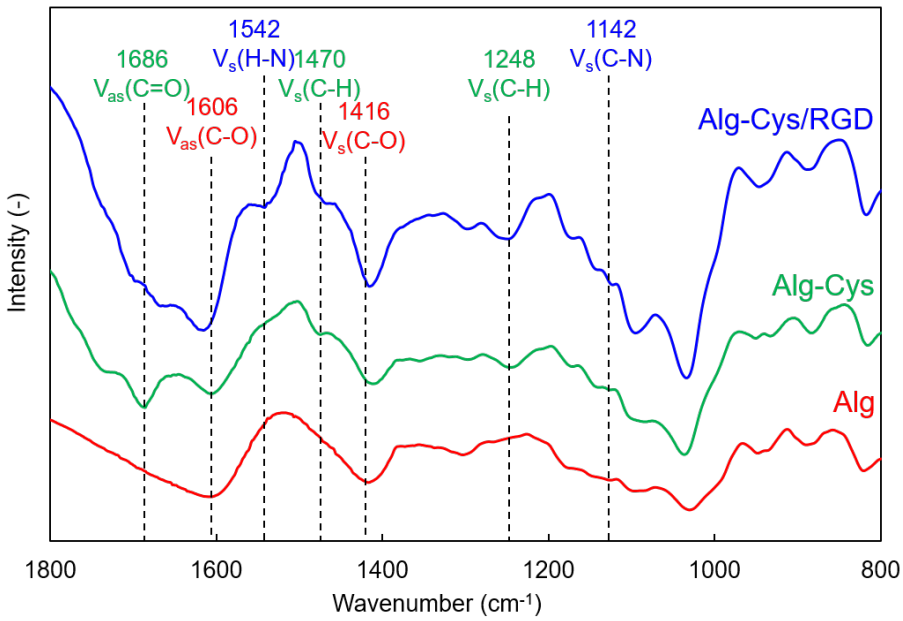

Figure S1. FTIR spectrum of cysteine and RGD peptide modified alginate.

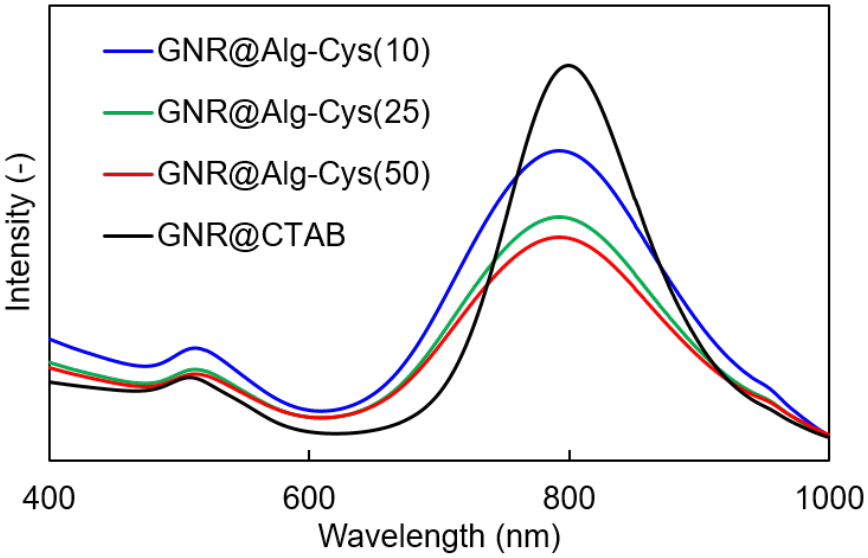

Figure S2. UV-visible absorption spectrum of GNR@Alg-Cys(X). X represents the amount (mg) of cysteine modified alginate used for replacing CTAB on 2 μg of GNR@CTAB.

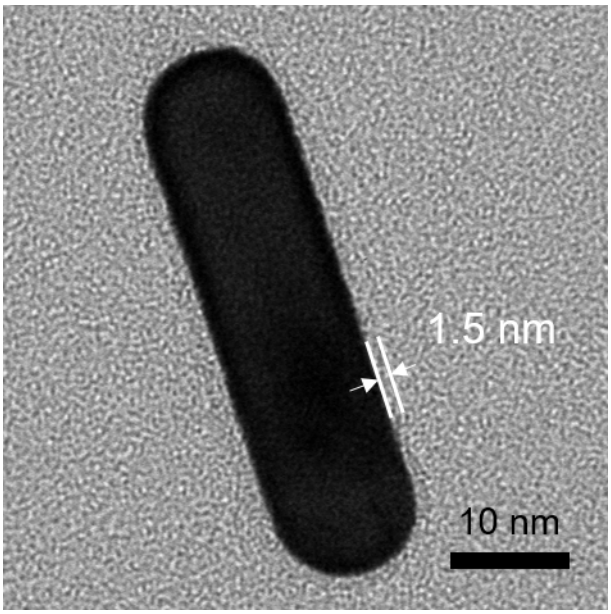

Figure S3 TEM image of GNR@Alg-Cys. A shell of Alg-Cys with 1.5 nm in thickness was observed on the GNR.

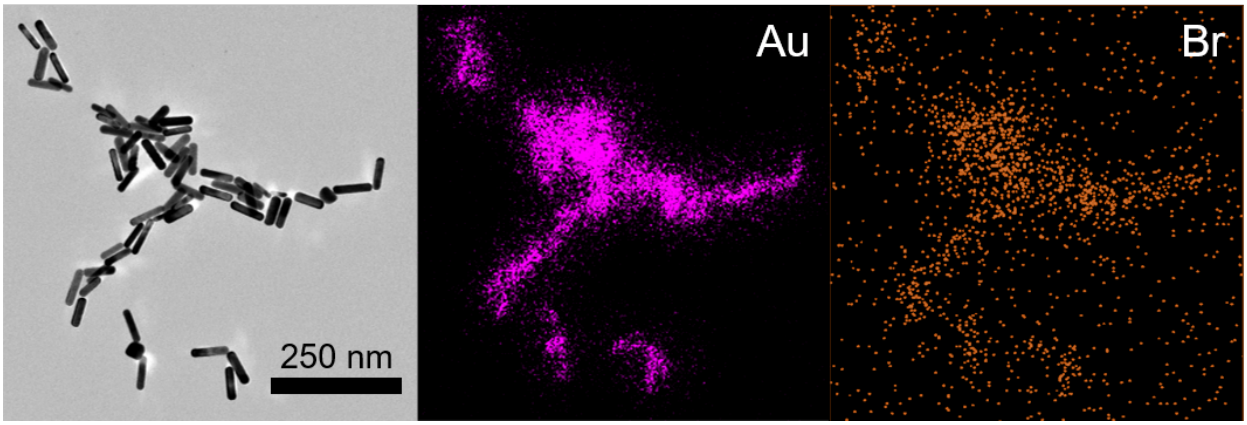

Figure S4. Element distribution of Au, Br on GNR@CTAB observed with TEM-EDX.

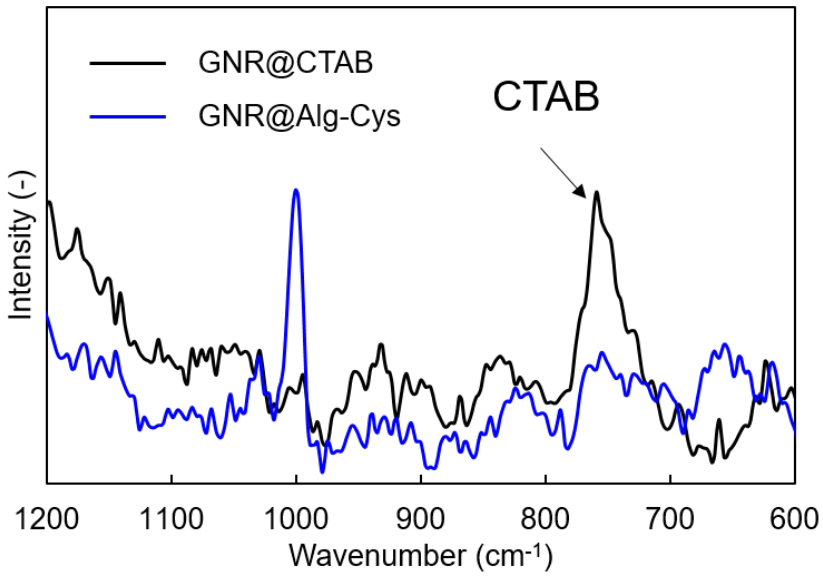

Figure S5. Raman spectrum of GNR@CTAB and GNR@Alg-Cys.

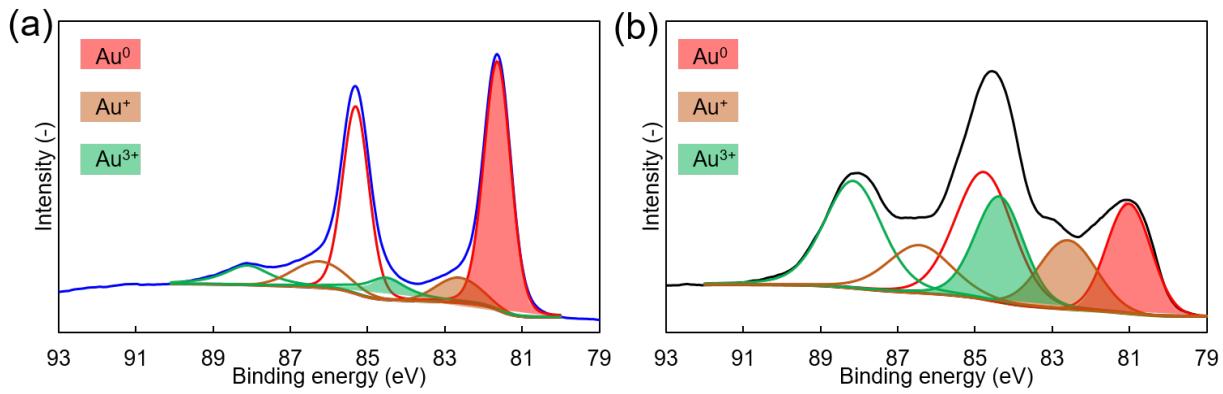

Figure S6. Integration area of Au^0 (red), Au^+ (brown), and Au^{3+} (green) state in (a) GNR@CTAB and (b) GNR@Alg-Cys.

Table S2 Summary of state of gold in GNR@CTAB and GNR@Alg-Cys.

	Atom percentage (%)*		
	Au^0	Au^+	Au^{3+}
GNR@CTAB	73.6	11.8	14.6
GNR@Alg-Cys	34.1	27.3	38.6

*: The atom percentage of each state is calculated by integration of the area of each state in XPS spectrum (Figure 2d and Figure S6)

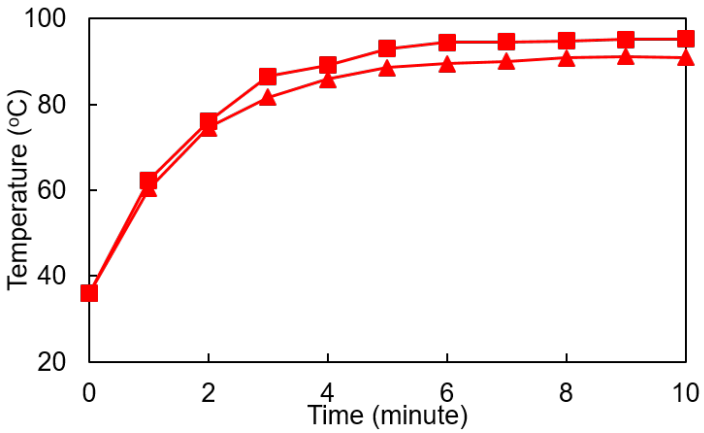

Figure S7. Time-dependent temperature profile of GNR@CTAB-containing PBS irradiated with diode laser (808 nm). Square stain represents the intensity of laser at 2 W/cm^2. Triangular stain represents the intensity of laser at 1.5 W/cm^2.