

Supporting Information for the manuscripts entitled
“Preparation and Antibacterial Activities of Silver Nanoparticle-Loaded Hydroxyapatite/Collagen
Bone-Like Nanocomposite”
authored by Masanori Kikuchi et al.

1. Details of the pseudo-first order model (PFO model) and the pseudo-second order model (PSO model) for adsorption equilibrium analysis.
2. Four major, two-parameter adsorption isotherm models
3. Supplementary Figure S1: Schematic drawing of donut-shaped HCM for antibacterial and cytotoxicity tests.
4. Supplementary Figure S2: Schematic explanation of (a) absorbance change obtained by periodical measurement, and (b) calibration curve plotting the time to reach the absorbance 1.0 and the inoculated number of bacteria.
5. Supplementary Figure S3: Powder X-ray diffraction (XRD) pattern of HAp/Col. Annotations are Miller indices for HAp. Collagen cannot be detected on XRD.
6. Supplementary Figure S4: Fourier-transformed infrared spectrum of HAp/Col. Small amount of carbonate group was substituted in PO_4^{3-} sites of HAp.

Five pages (including this cover page) with 4 figures.

1. Details of the pseudo-first order model and pseudo-second order model for absorption equilibrium time analysis

The pseudo-first order model (PFO model) [18] and the pseudo-second order model (PSO model) [19] described as following equations:

Kinetics curve of PFO model

$$Q_t = Q_e \{1 - \exp(-k_1 t)\} \dots (1)$$

Kinetics curve of PSO model

$$Q_t = \frac{k_2 Q_e^2 t}{k_2 Q_e t + 1} \dots (2)$$

where

t : time elapsed from the start of adsorption,

Q_t : adsorption amounts at each period ($\text{mg} \cdot \text{g}^{-1}$),

Q_e : equilibrium adsorption amount ($\text{mg} \cdot \text{g}^{-1}$),

k_1 : adsorption rate constant for PFO model (min^{-1}),

k_2 : adsorption rate constant for PSO model ($\text{g} \cdot \text{mg}^{-1} \cdot \text{min}^{-1}$).

Transform the above equations:

$$\ln(Q_e - Q_t) = \ln(Q_e) - k_1 t \dots (1)'$$

$$\frac{t}{Q_t} = \frac{1}{k_2 Q_e^2} + \frac{t}{Q_e} \dots (2)'$$

Based on these equations, t vs $\ln(Q_e - Q_t)$ and t vs t/Q_t were plotted to calculate linear fitting curves and parameters for the appropriate model.

2. Details of 4 major, two-parameter adsorption isotherm models

The details of 4 major, two-parameter adsorption isotherm models, Langmuir, Freundlich, Dubinin-Radushkevich (D-R), and Temkin, are described as follows [21]:

Langmuir isotherm model

$$Q_e = \frac{Q_0 K_L C_e}{1 + K_L C_e} \dots (3)$$
$$\frac{1}{Q_e} = \frac{1}{Q_0} + \frac{1}{Q_0 K_L C_e} \dots (3)'$$

Freundlich isotherm model

$$Q_e = K_f C_e^{\frac{1}{n}} \dots (4)$$
$$\ln Q_e = \ln K_f + \frac{1}{n} \ln C_e \dots (4)'$$

D-R isotherm model

$$Q_e = Q_s \exp(-K_{dr} \varepsilon^2) \dots (5)$$
$$\varepsilon = RT \ln \left(1 + \frac{1}{C_e}\right) \dots (6)$$
$$\ln Q_e = \ln Q_s - K_{dr} \varepsilon^2 \dots (5)'$$

Temkin isotherm model

$$Q_e = B \ln(A_T C_e) \dots (7)$$
$$B = \frac{RT}{K_T} \dots (8)$$
$$Q_e = B \ln A_T + B \ln C_e \dots (7)'$$

where

C_e : equilibrium concentration ($\text{mg} \cdot \text{L}^{-1}$)

Q_e : equilibrium adsorption amount ($\text{mg} \cdot \text{g}^{-1}$)

K_L : Langmuir constant ($\text{L} \cdot \text{mg}^{-1}$)

Q_0 : maximum adsorption amount of monolayer ($\text{mg} \cdot \text{g}^{-1}$)

K_f : Freundlich constant ($\text{L} \cdot \text{mg}^{-1}$)

n : heterogeneity in the adsorption process

K_{dr} : D-R constant ($\text{mol}^2 \cdot \text{kJ}^{-2}$)

ε : the Polanyi potential ($\text{kJ} \cdot \text{mol}^{-1}$)

Q_s : theoretical saturation capacity ($\text{mg} \cdot \text{g}^{-1}$)

R : universal gas constant ($8.314 \text{ J} \cdot \text{mol}^{-1} \cdot \text{K}^{-1}$)

T : Kelvin temperature (K)

A_T : the equilibrium binding constant ($\text{L} \cdot \text{g}^{-1}$)

B : the constant related to the heat of adsorption ($\text{J} \cdot \text{mol}^{-1}$)

K_T : Temkin constant

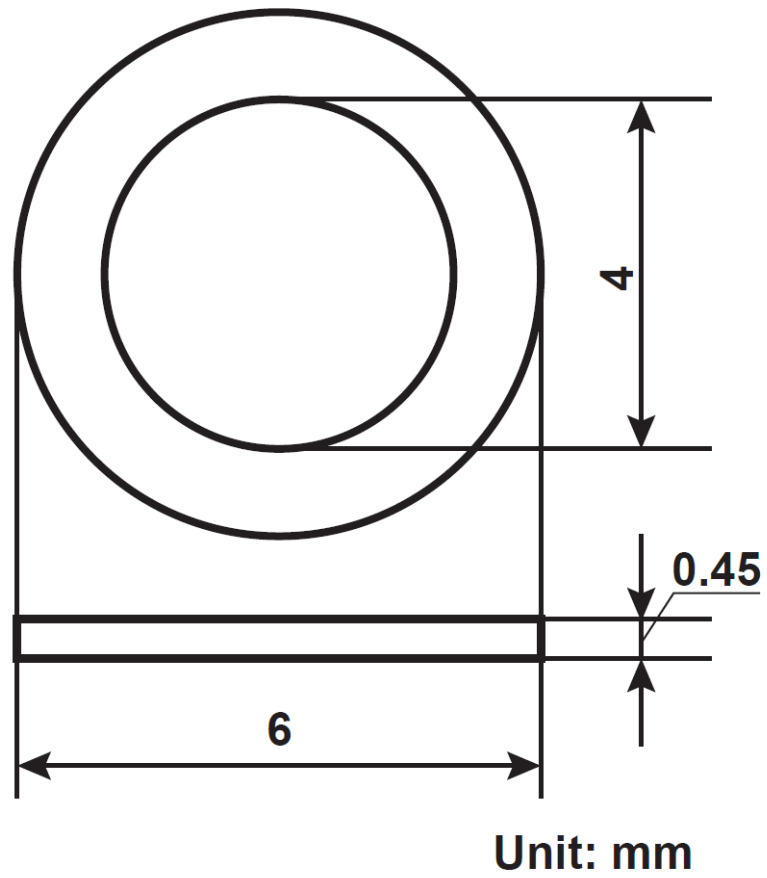


Figure S1. Schematic drawing of donut-shaped HCM for antibacterial and cytotoxicity tests.

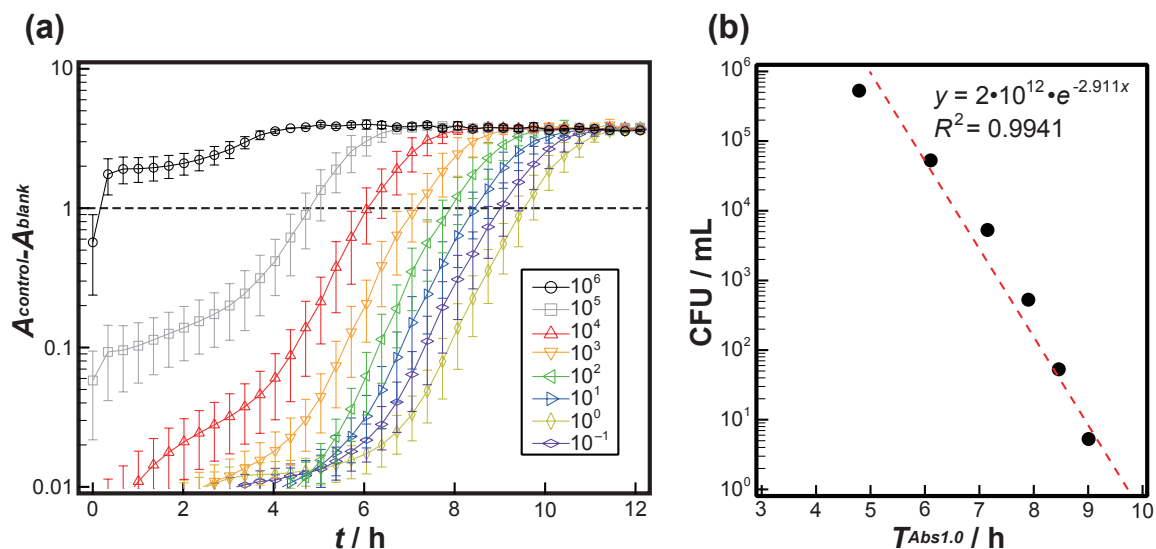


Figure S2. Schematic explanation of (a) absorbance change obtained by periodical measurement, and (b) calibration curve plotting the time to reach the absorbance 1.0 and the inoculated number of bacteria.

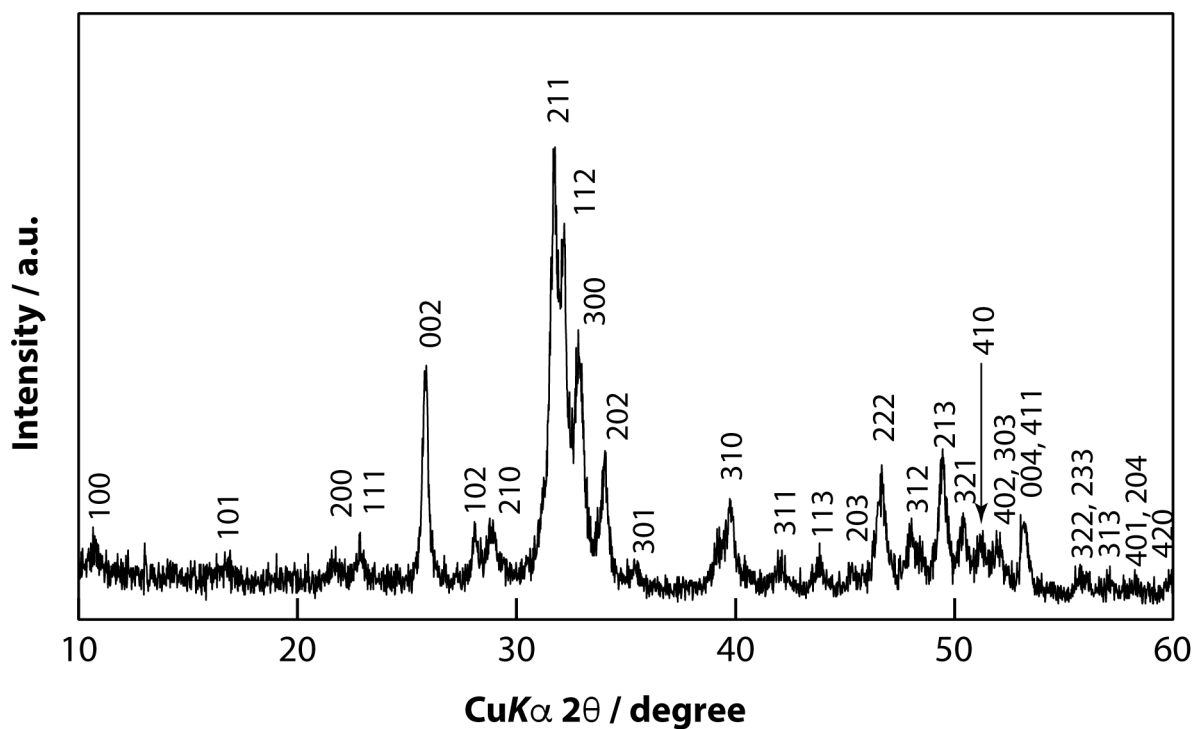


Figure S3. Powder X-ray diffraction (XRD) pattern of HAP/Col. Annotations are Miller indices for HAP. Collagen cannot be detected on XRD.

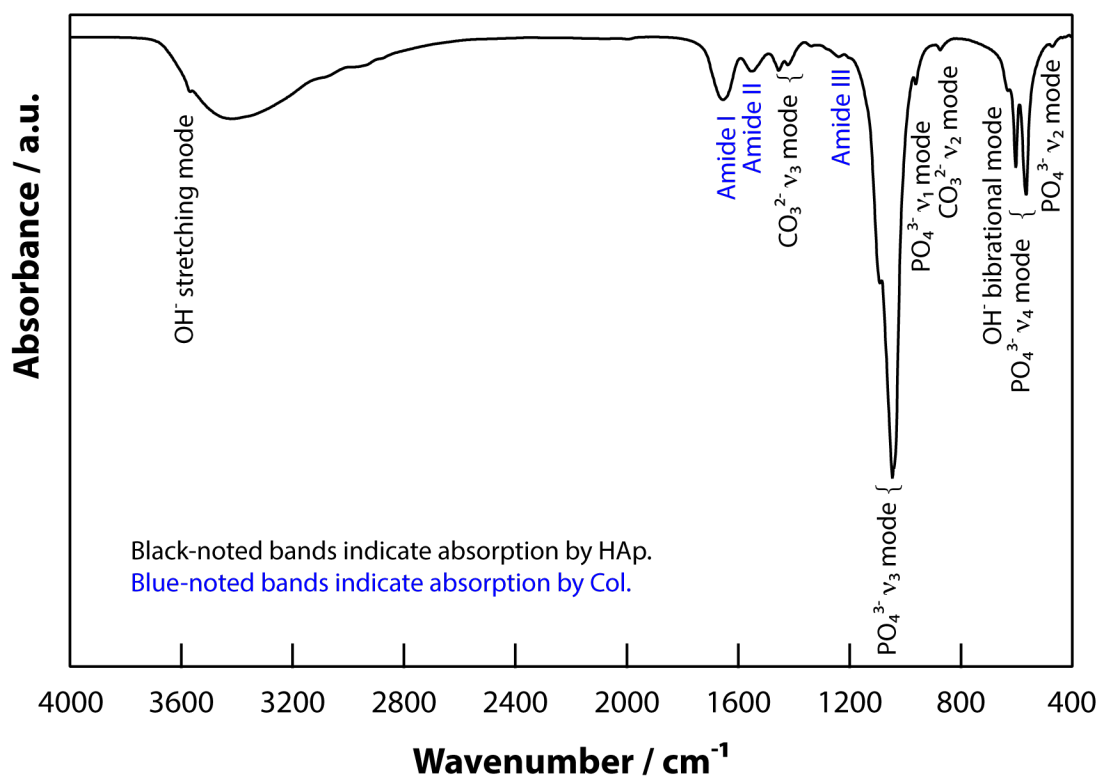


Figure S4: Fourier-transformed infrared spectrum of HAp/Col. Small amount of carbonate group was substituted in PO₄³⁻ sites of HAp.