Title:
Supramolecular Nanotube endo-Sensing for a Guest Protein

Authors:
Naohiro Kameta,* Mitsutoshi Masuda, Go Mizuno, Nahoko Morii, and Toshimi Shimizu*

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1. **Molecular packing analysis of the Alexa-nanotube by IR spectroscopy**

IR spectrum of the Alexa-nanotube indicates two peaks at 1420 and 1026 cm$^{-1}$ as shown in Figure S1. The two bands are observable in the CH deformation and skeletal vibration bands of polyglycine. This means that the triglycine of 1 and 2 in the Alexa-nanotube form intermolecular hydrogen-bonding similar to the polyglycine-II-type hydrogen-bond networks of polyglycine (Figure S2). Pseudo hexagonal hydrogen-bond networks should induce the parallel molecular packing within single monolayer of the Alexa-nanotube.

![Figure S1. IR spectrum of the lyophilized Alexa-nanotube.](image)

![Figure S2. Polyglycine-II hydrogen-bond networks of triglycine.](image)
The \( r(\text{CH}_2) \) rocking vibration band reflects the lateral chain packing of the oligomethylene spacer in 1 and 2, the so-called “subcell structure”, supported the parallel molecular packing. IR spectrum shows a single sharp peak at 719 cm\(^{-1}\), indicating a triclinic parallel (T\(_//\)) structure (Figure S3).

![Subcell structure of the oligomethylene spacer of 1 and 2.](image)

All results suggest that the Alexa-nanotubes consist of a single monolayer with parallel molecular packing, and have different inner and outer surfaces covered with amino and glucose groups, respectively. Consequently, the Alexa moiety as a recognition probe is located on the inner surface of the nanotubes without exception.

11. **Absorption and fluorescence spectroscopy of the Alexa-nanotube and GFP**

Fluorescence band of the GFP partly overlapped with the absorption band of the Alexa-nanotube (Figure S4). Therefore, if GFP can approach the Alexa moiety within a few nm in the hollow cylinder structure of the nanotube, the fluorescence resonance energy transfer (FRET) should occur from GFP to the Alexa moiety. The fluorescence intensity of GFP (510 nm) decreased with upon addition of the Alexa-nanotube at pH 6.8, while a new band (570 nm) corresponding to the Alexa appeared at the same time. This phenomenon is ascribable to the FRET from the encapsulated GFP to the Alexa moiety on the inner surface of the nanotube hollow cylinder. Similar spectral change hardly occurred at pH 8.5. Protonation state of the amino groups on the inner surface of the Alexa-nanotube strongly influences the encapsulation of the negatively charged GFP.
Figure S4. Absorption (dotted line) and fluorescence (solid line) spectra of GFP (green color) and the Alexa-nanotube (pink color) dispersed solutions.

Figure S5. Fluorescence spectra of GFP in the absence (dotted line) and the presence (solid line) of the Alexa-nanotube under different pH conditions in the solutions. Excitation wavelength is 450 nm.