Effect of Molecular Distortion on the Optical Properties of Carotenoid-Based Nanoparticles

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Certain vegetables and fruits produce carotenoid compounds during their ripening process, which gives them vivid yellow, orange, or reddish colors. The optical properties of carotenoids are of practical importance in the food industry as well as in nature, where they are widely used as natural pigments in various food products. Unlike typical organic pigments, which have a rigid, aromatic-based molecular structure, carotenoids have flexible molecular structures derived from polyene skeletons (**Fig. 1a**: *β*-carotene is one of the carotenoids found in carrots). This means carotenoid molecules are easily distorted in response to stress and change their properties. Interestingly, the absorption spectrum of carotenoid nanoparticles obtained by reprecipitation is known to be blue-shifted compared to that of bulk crystal (**Fig. 1b**). In this study, the optical properties of carotenoid-based nanoparticles was investigated through detailed structural analysis where I predicted that the structural factor of molecular distortion plays an important role in influencing carotenoid optical properties.

Carotenoid-based NPs were obtained with < 100 nm in diameter by reprecipitation method.[1] Using transmission electron microscopy, electron diffraction analyses, and powder X-ray diffraction measurements, it is revealed that obtained nanoparticles comprised two domains: a crystalline domain and an amorphous domain (**Fig. 1c**). Raman spectroscopy was then used to evaluate the effective π-conjugation length of the carotenoids. It is known that the peak position of the Raman band assigned to the C=C stretching vibration (ν_1) correlates with the length of the π-conjugation length of the carotenoid polyene chain.[2] Detailed analysis of ν_1 Raman band showed that NPs include the molecules that shortened effective π-conjugation in their amorphous domain, suggesting the molecules are distorted (**Fig. 1c**). Furthermore, I revealed a correlation between the absorption spectra and the extent of carotenoids distortion - labelled effective π-conjugation lengths. This led to the conclusion that molecular distortion strongly affects optical properties.

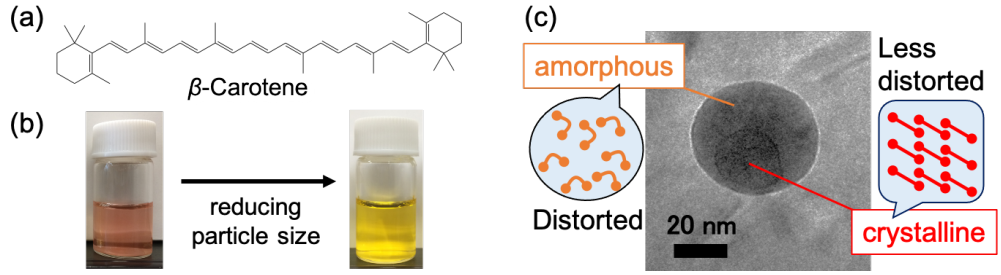

Fig. 1 (a) Chemical structure of *β*-carotene (b) *β*-carotene particles dispersion that change color as particle size reduction (c) *β*-carotene nanoparticle taken by a cryo-transmission electron microscope

References: 1) H. Kasai *et al.*, *Jpn. J. Appl. Phys.*, **1992**, *31*, L1132. 2) J. C. Merlin, *Pure & Appl. Chem.*, **1985**, *57*, 785.