Inclusion Structure of α-cyclodextrin with surfactant in dilute aqueous solutions

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The cyclic oligosaccharide, cycrodextrin, has the ability to incorporate various organic molecules into its hydrophobic cavity. The α-cycrodextrin(α-CD) which is composed of six sugars can include hydrophobic part of surfactant such as sodium dodesyl sulfate (SDS) in aqueous solution. In this experiment the small-angle X-ray scattering (SAXS) method was carried out to observe the inclusion structure in dilute solutions.

The SAXS experiment was performed at BL40B2. The optical system was adjusted as 1Å for wave length of incident X-ray and 1 m for camera length. The scattering intensity is obtained by calculating circular average from two-dimensional data detected with imaging plate (IP).

Figure 1 shows SAXS profiles ($I(q)$ vs. q, where $I(q)$ is scattering intensity and q is the magnitude of scattering vector) from α-CD with and without SDS. The maximum was observed around higher q region, where the peak position shifted to smaller q by adding SDS. This behavior was considered to be due to the inclusion of SDS to α-CD. The radius of gyration Rg is estimated as Rg = 5.8 Å for SDS = 0 mg/ml, Rg = 6.4 Å for SDS = 0.21 mg/ml, and Rg = 6.9 Å for SDS = 0.71 mg/ml, respectively. The SDS molecule is speculated to include with one or two α-CD molecules.

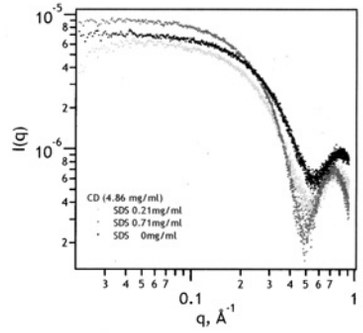

Figure 1. SAXS profiles from α-CD with and without SDS in aqueous solutions.

Solution Structure and Hydration States of Proteins by Precise Analysis of X-ray Scattering Profiles in the Wide Q-range

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[Introduction]

The solution x-ray scattering (SXS) method gives information on the global structure of solute molecules. Guinier and Kratky analyses of proteins at small K<3 nm^{-1} have yielded their molecular images in the nonnative state. [1] As the highly accurate measurement of SXS profiles in the medium to large K region of 3-10nm^{-1} has become possible by advances in experimental techniques, it is expected that more detailed structural information will be obtained in future. In this K region, however, hydrating water has significant contribution to SXS profiles, which needs to be evaluated quantitatively. We estimated SXS profiles of native proteins using an accurate hydration model [2] obtained from their MD simulation to compare with experiment. Highly accurate SXS measurements to large K region have also been made on nonnative proteins.

[Method]

SXS measurements have been made using Spring-8 BL40B2. The detector is an imaging plate. The sample-to-detector distance is 1 m and the x-ray wavelength is 0.1 nm, which enables us to have SXS profiles to K= 9 nm^{-1}. To minimize radiation damage, a flow cell was used with the flow rate of 3 ˙ / . Horse myoglobin was taken as sample protein. SXS measurements were made on holo-myoglobin in the native state and apo-myoglobin in each of the native, molten globule (MG), acid unfolded (AU) and acid MG states.

[Result]

The experimental SXS profile for native holo-myoglobin and the calculated one with the accurate hydration model were found to coincide with each other over the whole K<9 nm^{-1}. It confirms the validity of our hydration model. We obtained also experimental profiles for the MG and AU states. Analysis of these data using the molecular modeling method of the nonnative state and the hydration model will give us detailed information on the nonnative structure of myoglobin.

[Reference]

1) M. Kataoka et al., *Fold. Des.*, 1 (1996) R107-114.

2) Y. Seki et al., *Biophys. Chem.*, 95 (2002) 235-252.