

Structural study of hNck2 SH3 domain protein by X-ray solution scattering IV. Structural analysis of hNck2 SH3 domain at pH 2 and pH 8: non-native α -helix-rich monomer and native dimer

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Introduction

hNck2 SH3 domain is a protein which takes β -structure at the native state. Liu and Song reported [1] that the protein forms non-native α -helix-rich structure below pH 2 based on NMR spectroscopy.

We have shown in the series of reports that hNck2 SH3 domain protein takes native β -structured state at pH 6 and takes dimer at the concentration higher than 1 mg/mL [2], and at low pH, the protein takes mainly monomer even at 3 mg/mL [3]. This acid-stable monomer is rich in α -helix and non-compact [4].

In the present report, we show proposed structure of the protein at pH 2 and pH 8 from DAMMIN analysis [5].

Experimental and Calculation

X-ray solution scattering experiments were done at BL 6A. Details of the experimental procedures are shown elsewhere [3]. Protein concentration was 3 mg/mL. At this concentration, protein takes monomer at pH 2 and dimer at pH 8 from $I(0)$ analysis of the X-ray solution scattering data [3].

Structural calculations were done for the scattering data at pH 2 and pH 8 by using DAMMIN program [5].

Results

Scattering patterns of hNck2 SH3 domain protein at pH 2 and pH 8 are shown in Figure 1.

Figure 2 shows calculated structures at pH 2 and pH 8. At pH 2, an elongated structure was obtained. As the Kratky plot of this state did not show a peak, but a plateau shape, the structure at pH 2 is not compact. As the state is richer in α -helix than the native state, the hNck2 SH3 domain protein takes non-compact, but non-random coiled, i.e. C-state which Yamada suggested for equine beta-lactoglobulin [6]

At pH 8, the protein takes ellipsoidal structure. The volume of the structure at pH 8 is found to be almost twice as large as that at pH 2, which also supports the structure below pH 2 is monomer and the structure above pH 4 is dimer.

References

[1] Liu & Song (2008) *Biophys. J.* 95, 4803-4812.

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[4] Matsumura *et al.* (2012) This proceedings, III.

[5] Svergun (1999) *Biophys. J.* 76, 2879-2886.

[6] Yamada *et al.* (2005) *J.Mol.Biol.* 350, 338-348.

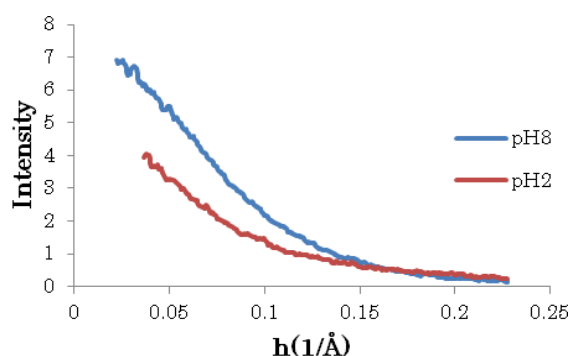


Figure 1. Scattering intensity of hNck2 SH3 domain at pH 2 and pH 8. Non-linear small angle region were cut for DAMMIN calculation.

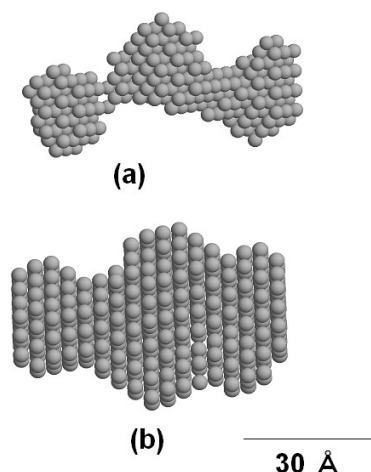


Figure 2. Calculated structure of hNck2 SH3 domain by DAMMIN program. (a) pH 2 (b) pH 8

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