

SAXS_MD 法による srcSH3ドメイン蛋白の α -ヘリックスに富むフォールディング中間体の構造解析

Structural analysis of α -helix-rich intermediate of srcSH3 domain protein on its folding pathway by SAXS_MD

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SrcSH3 forms α -helix-rich intermediate in the early stage of folding pathway¹⁾. The estimated fraction of α -helix is 25% from circular dichroism measurement. Time-resolved X-ray solution scattering experiment was also done. Radius of gyration of the intermediate is 18.5Å, much smaller than that of the unfolded state (27Å) and larger than that of the native state (14.6Å). We calculated molecular structure with atomic coordinate by SAXS_MD²⁾ program. Initial extended structure moved to fit X-ray solution scattering data and reached to shrink structure, but without α -helix. We arranged to make 25% α -helix on to the shrunk structure (Fig.1). This α -helix-rich structure shows better fitting to the X-ray solution scattering data than the shrunk non-helical structure. Energy calculation also shows that this structure is stable. This α -helix-rich structure possibly expresses the folding intermediate of src SH3.

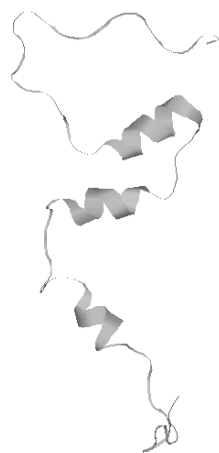


Fig. 1 α -helix-rich structure

- 1) Li *et al.* (2007) *Biochemistry* 46, 5027-5082
- 2) Kojima *et al.* (2004) *J. Appl. Cryst.* 37, 103-109