An Oblate Shape of Ca\(^{2+}\) (and Zn\(^{2+}\))-bound S100A3 Homotetramer

Kenji KIZAWA\(^1\), Yuji JINBO\(^2\), Takafulmi INOUE\(^1\), Yoshinobu IZUMI\(^2\)*

\(^1\)Basic Research Laboratory, Kanebo Cosmetics Inc., Odawara 250-0002, Japan
\(^2\)Graduate School of Science & Eng., Yamagata Univ., Yonezawa, Yamagata 992-8510, Japan

**Introduction**

S100A3, of which Arg-51 is specifically converted to citrulline by Ca\(^{2+}\)-dependent peptidylarginine deiminases (type III), assembles a homotetramer within hair cuticular cells [1]. Its Cys-rich C-terminal domain reported to bind two Zn\(^{2+}\) ions [2], however its structural and functional in the Ca\(^{2+}\)-dependent tetramerization is still unknown. This study aimed to elucidate Ca\(^{2+}\) (and Zn\(^{2+}\))-bound tetrameric architecture in solution by small-angle X-ray scattering (SAXS) analyses.

**Materials and methods**

Dimer to tetramer ratio of S100A3 and R51A (a mutated protein analogous to the citrullinated form), and overall shape in Ca\(^{2+}\) (and Zn\(^{2+}\))-containing solution were evaluated using the SAXS measurement at BL-10C [3].

**Results and discussion**

Mol fraction of S100A3/R51A tetramer was calculated from \(M_n\) determined by SAXS data with the Guinier approximation. S100A3/R51A dimers converted to tetramers up to ~70% even at 100 mM Ca\(^{2+}\). Fluorescent titration revealed that affinities to either Ca\(^{2+}\) or Zn\(^{2+}\) of S100A3 were mutually increased by the concurrent heterotrophic ion. In the presence of Zn\(^{2+}\), R51A more efficiently assembled a homotetramer with 1mM Ca\(^{2+}\) [4].

**References**


*yizumi@yz.yamagata-u.ac.jp