Revealing the Solution Conformation and Hydration Structure of Type I Tropocollagen using X-ray Scattering and Molecular Dynamics Simulation

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Hydration plays a crucial role in regulating the dispersion behavior of biomolecules in water, particularly in how pH-sensitive hydration water network forms around proteins. This study investigates the conformation and hydration structure of type-I tropocollagen using small- and wide-angle X-ray scattering (SWAXS) and molecular dynamics (MD) simulations. SWAXS data for type-I tropocollagen in a pH 2 solution were collected at the 3.0 GeV Taiwan Photon Source -National Synchrotron Radiation Research Center, employing an integrated online size exclusion chromatography (SEC) system alongside UV-Vis absorption and refractive index spectrometers. [1]. The SWAXS data in the range of 0.002 – 0.1 Å^{-1} were fitted using the worm-like chain (WLC) model in conjunction with power law scattering (q^{-2} and q^{-1}), as illustrated in Figure 1. The results reveal that tropocollagen exhibits a significant softening conformation in solution, transitioning from its rod-like structure in tissues to a worm-like conformation, characterized by a reduced radius of gyration of 50 nm and a persistent length of 34 nm. The higher q data in the range of 0.06 – 2.5 Å^{-1}, characterized by two humps at q_0 and q_1, were calculated using the GROMACS-SWAXS with the MD simulation of a truncated tropocollagen (~ 13 nm in length) [2]. The SWAXS calculations further establish a hydration water network characterized by a 2.8Å free-water exclusion zone where water molecules are all hydrogen-bonded to the densely distributed polar groups on the tropocollagen surfaces. These first-layer water molecules are bridged by outer water molecules extending up to 4 Å from the protein surfaces, forming an extensive hydration shell that encapsulates the protein.

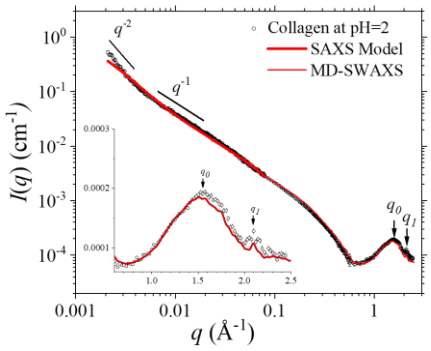

Figure 1: The experimental SWAXS data for the tropocollagen solution at pH 2 are well characterized by power law scattering, fitting to the worm-like chain (WLC) model, and GROMACS-SWAXS calculations across a wide q range (0.002 - 2.5 Å^{-1}). The inset highlights the two humps of q_0 and q_1.

References

[1] O. Shih *et al.*, *J. Appl. Cryst.*, **55**, 340–352 (2022).
[2] P.-C Chen *et al.*, *Biophys. J.* **107**, 435–447 (2014).

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