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Solvation Shell Structure of Proteins probed by Small- and Wide-Angle X-Ray Scattering

Small- and wide-angle X-ray scattering (SWAXS) data provides information about the shape and size of biomacromolecules in solution. The newly developed BioSAXS endstation at the beamline 13A of the Taiwan Photon Source features an in-vacuum SWAXS detecting system comprising two area detectors (Eiger X 9M/1M) and an online size-exclusion chromatography system incorporated with several optical probes, including UVvis absorption spectrometer and refractometer. The instrumentation allows simultaneous SAXS and WAXS data collection with a high signal-to-noise ratio, enhancing structural studies of biomolecules by accessing finer details of solution structures. Here we tested a model protein BSA with two common denaturants: urea and guanidinium chloride (GdmCl). The intradomain interaction loss is clear around the middle q region. The high q peak (~1.5 Å-1) was previously assigned to the secondary structure but is still present when the protein is fully denatured. We showed how the solvation structure changes correlate with the high q peak change and discussed the different outcomes from urea and GdmCl, suggesting a dissimilar denaturation mechanism.

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