Monitoring Molecular Metamorphosis using Wide-angle Solution Scattering Data

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The structure motifs of proteins and other biological macromolecules have characteristic distributions of interatomic distances that produce features buried within the x-ray scattering pattern from that molecule in solution. We have demonstrated that wide-angle x-ray solution (WAXS) scattering contains rich details of the secondary, tertiary and quaternary structure of multiple classes of proteins. Uses to date include the observation of ligand-induced structural cdhanges and the monitoring of fold stages during chemical and radiation-induced protein denaturation. WAXS scattering patterns obtained at high flux third generation synchrotron beam lines are not only sensitive to protein conformational states, but the scattering patterns generated can be quantitatively compared to data calculated from detailed structural models derived from crystallographic data.

Our group has used the 18ID beamline at the Advanced Photon Source to study various classes of molecular transitions of proteins and nucleic acids. WAXS is shown here to be a sensitive reporter for such phenomena as radiation-induced quaternary structure breakdown, molecular crowding, folding transition states and changes in structure induced by ligand-binding. As such, WAXS has great potential as a complementary methodology to augment the structural information gleaned from static crystalline arrays.

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