Solution Bio-SAXS in High Throughput at SIBYLS

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Structural analysis by small angle X-ray scattering of biological macromolecules efficiently enables the characterization of shape and assembly for nearly any purified target. Crystallography has provided a deep and broad survey of macromolecular structure. Shape and assembly from SAXS in combination with available structures is often enough to answer critical mechanistic questions both enhancing the value of a structure and identifying other high impact crystallographic projects. Moreover, SAXS is a solution based technique, sample requirement are modest and compatible with many other biophysical methods. The SIBYLS beamline is a joint SAXS and crystallography endstation. The SAXS portion of the SIBYLS beamline, designed in part by Hiro Tsuruta, has been in operation for 5 years. A central motivation for building SIBYLS were experiments conducted in collaboration with Hiro on the DNA repair enzyme RuvB. Here we present our high throughput SAXS data collection and analysis pipeline as applied to DNA repair targets, and metabolic pathways. Our goals of metabolic engineering and understanding protein mediated reactions rely on knowing the shape and assembly state of reactive complexes under an array of conditions. Given the number of gene products involved in metabolic networks, SAXS will play an important role in characterizing the structure of each individually, in complex with partners, and in various contexts. SAXS is well positioned to efficiently bridge the rapid output of bioinformatics and the relatively slow output of high resolution structural techniques.