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Automated structural modeling in biological small-angle X-ray scattering

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Small-angle X-ray scattering (SAXS) experiences a renaissance in the studies of macromolecular solutions allowing one to study the structure of native particles and complexes and to rapidly analyze structural changes in response to variations in external conditions. New high brilliance sources and novel data analysis methods significantly enhanced resolution and reliability of structural models provided by the technique (Graewert & Svergun, 2013). Automation of the experiment, data processing and interpretation make solution SAXS a streamline tool for large scale structural studies in molecular biology. The recent developments will be presented including robotic sample changers, pipelines for data processing, computation of structural parameters and ab initio models, classification of the folding states of macromolecules. A prototype of an expert systems allowing for automated generation and assessment of structural models will be considered. A synergistic use of SAXS with the high resolution methods like crystallography and NMR, but also with complementary biophysical and biochemical techniques will be discussed. The problems of validation of SAXS-generated models, and the use of data quality assessment tools for the deposition of the models and experimental data will be discussed. Further perspectives of the hybrid applications of SAXS with other techniques in structural biology will be outlined.

[1] *Graewert MA, Svergun DI. (2013) Impact and progress in small and wide angle X-ray scattering (SAXS and WAXS). Curr Opin Struct Biol. 23:748-54.*

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