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Keynote 6, Dr. Andrey Gruzinov: Small-angle X-ray scattering (SAXS) for integrative structural biology

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Small-angle X-ray scattering (SAXS) is a powerful method in the studies of solutions of biological macromolecules and nanostructured systems [1] allowing one to analyze the structure of native particles and complexes and to rapidly assess structural changes in response to variations in external conditions. Dedicated high brilliance synchrotron beamlines and novel data analysis methods [2] significantly enhanced resolution and reliability of the structural models provided by SAXS. Very important is the ability of SAXS to quantitatively characterize complicated systems and mixtures in native environments and to see the biomolecules in action by rapidly observing responses to changing physical and chemical conditions (e.g. upon pH or temperature changes, ligand binding etc).

Given the limited information content in the scattering data, robust data analysis and modelling methods are of major importance for broad applications of solution SAXS in biology. To reduce the ambiguity of interpretation, SAXS is often combined with other structural methods like crystallography, NMR and electron microscopy, and also with computational, biophysical and biochemical techniques to build hybrid models. In classical applications, SAXS generally yields low resolution quaternary structure but, very importantly, the method can also help to analyze equilibrium mixtures and to visualize flexible portions of the structures, not seen by the high resolution methods.

In the present talk, modern methods for SAXS data analysis will be presented and illustrated by applications to characterize structures and conformational transitions of biological macromolecules in solution. Recent developments including, in particular, in-line chromatography approaches [3] will be elucidated and perspectives of the synergistic use of SAXS for integrative modeling utilizing complementary methods will be discussed.

Presenter(s) : GRUZINOV, Andrey (EMBL c/o DESY, Hamburg, Germany)

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