ISSRNS 2010: Abstracts / Synchrotron Radiation in Natural Science Vol. 9, No. 1 – 2 (2010)

STRUCTURAL STUDIES OF BIOLOGICAL MACROMOLECULES IN SOLUTION USING SYNCHROTRON SMALL-ANGLE X-RAY SCATTERING

M. Roessle [*] and D.I. Svergun

European Molecular Biology Laboratory, Hamburg Outstation c/o DESY, Notkestr. 85, D22603 Hamburg, Germany

Keywords: x-ray scattering, quaternary structure, remote experiments

**) e-mail: svergun@embl-hamburg.de*

Small-angle X-ray scattering (SAXS) experiences a renaissance in the studies of solutions of biological macromolecules. SAXS is a low resolution (1-2 nm) structural method, which is applicable to native states of macromolecules in solution providing information about the overall structure and structural transitions. The method covers a broad range of sizes, from individual macromolecules to multi-domain proteins and large macromolecular assemblies. High brilliance synchrotron sources and novel data analysis methods [1] significantly enhanced resolution and reliability of structural models provided by the technique. Emerging automation of the synchrotron SAXS experiment, data processing and interpretation make solution SAXS a streamline tool for large scale structural studies in molecular biology. The method provides low resolution macromolecular shapes *ab initio* and is readily combined with other structural and biochemical techniques in multidisciplinary studies. In particular, rapid validation of predicted or experimentally obtained high resolution models in solution, identification of biologically active oligomers and addition of missing fragments to high resolution models are possible. For macromolecular complexes, quaternary structure is analyzed by rigid body movements/rotations of individual subunits. Recent developments made it possible also to quantitatively characterize flexible macromolecular systems, including intrinsically unfolded proteins. The novel methods will be illustrated by advanced applications of synchrotron SAXS to solutions of biological macromolecules. Possibilities of remote and high throughput operation using synchrotron radiation combined with automated sample changers and data analysis pipelines [2] will be presented.

References

[1] M.V. Petoukhov, D.I. Svergun, "Analysis of X-ray and neutron scattering from biomacromolecular solutions," *Curr. Opin. Struct. Biol*. **17** (2007) 562–571.

[2] A.R. Round, D. Franke, S. Moritz, R. Huchler, M. Fritsche, D. Malthan, R. Klaering, D.I. Svergun and M. Roessle, "Automated sample-changing robot for solution scattering experiments at the EMBL Hamburg SAXS station X33", *J. Appl. Crystallogr.* **41** (2008) 913–917..