MS.51.1

Acta Cryst. (2008). A**64**, C91

Joint use of SAXS and SANS with high resolution methods for macromolecular solutions

Dmitri I. Svergun[1,2]
[1]EMBL, [2]Institute of Crystallography, Russian Academy of Sciences, Leninsky pr. 59, 117333 Moscow, E-mail：svergun@embl-hamburg.de

Small-angle scattering of X-rays and neutrons (SAS) allows one to study the structure of native particles in nearly physiological solutions and to analyse structural changes in response to variations in external conditions. The scattering data bear information about the overall shape and internal structure at a resolution of 1-2 nm. The method is applicable to a broad range of sizes, from individual macromolecules to multi-domain proteins and large macromolecular assemblies. Recent progress in instrumentation and especially development of novel data analysis methods [1] significantly enhanced resolution and reliability of structural models provided by the technique and made SAS a useful complementary tool to high resolution methods, including large scale structural studies. In particular, rapid validation of crystallographic models in solution, identification of biologically active oligomers and addition of missing fragments to high resolution models are possible. For macromolecular complexes, quaternary structure can be analyzed in terms of rigid body movements/rotations of high resolution models of the individual subunits of domains. Advanced applications of SAS to macromolecular solutions will be presented including, in particular, ab initio low resolution structure determination, rigid body refinement, contrast variation studies of complexes and quantitative analyses of flexible macromolecules.
[1] Petoukhov, M.V. & Svergun, D. I. (2007) Curr Opin Struct Biol. 17, 562-571

Keywords: small-angle scattering, macromoleclar structure, rigid body refinement

MS.51.2

Acta Cryst. (2008). A**64**, C91

Additivity, redundancy, and complementarity between structural information from NMR and SAXS data

Masaki Kojima[1], Yasumasa Morimoto[2], Takashi Nakagawa[2], Shigeru Yanagi[2], Hiroshi Kihara[3], Takamasa Nonaka[1]
[1]Iwate Medical University, School of Pharmacy, 2-1-1 Nishitokuta, Yahaba, Iwate, 028-3694, Japan, [2]Tokyo University of Pharmacy and Life Science, 1432-1 Horinouchi, Hachioji, Tokyo, 192-0392, Japan, [3]Kansai Medical University, 18-89 Uyama-Higashi, Hirakata, Osaka, 573-1136, Japan, E-mail：mkojima@iwate-med.ac.jp

At present protein structure in solution is determined by restrained molecular dynamics with distance restraints mainly derived from NMR. Although the small-angle X-ray scattering (SAXS) method also confers the structural information, its content is too small to determine the structure by itself. We previously developed a new algorithm that refines the protein structure by restrained molecular dynamics with SAXS constraints[1)]. In the present study we performed the protein structure calculation by restrained molecular dynamics with both NMR and SAXS constraints, in order to elucidate the essential structural information that defines the protein architecture.
We used RNase T1 as a model protein, which has already been determined by NMR alone[2)]. At first we added SAXS constraints ($h < 0.3$ Å^{-1}) into the original NMR-derived restraints for the calculation. The quality of the structure ensemble was significantly increased. Next we removed the original NMR restraints randomly in order to estimate the redundancy among the NMR-derived information. The essential topology of the resultant structures was hardly changed until the restraints were reduced below the half. Then we added the SAXS constraints into the remaining NMR restraints to expect they could complement the lost structural information. However, the structure was not recovered properly. By removing various types of structural information exclusively from the original NMR data set, we investigated whether the SAXS constraints could complement some kinds of structural information. The results showed that the SAXS could complement the tertiary structure to some extent while it could not secondary structure.
1) Kojima et al. (2004) J. Appl. Cryst. 37, 103-109
2) Hatano et al. (2003) Biol. Chem. 384, 1173-1183

Keywords: SAXS, NMR, molecular dynamics

MS.51.4

Acta Cryst. (2008). A**64**, C91−92

Time-resolved X-ray scattering studies on bacteriophage assemblies

Hiro Tsuruta[1], Roman Tuma[2,3], Kenneth H French[2], Peter E Prevelige[2], Kelly K Lee[4], Lu Gan[4], Crystal Moyer[5], James F Conway[6], Robert L Duda[5], Roger W Hendrix[5], Alasdair C Steven[7], John E Johnson[4]
[1]Stanford University, SSRL/SLAC, 2575 Sand Hill Rd MS69, Menlo Park, CA, 94025-7015, USA, [2]University of Alabama at Birmingham, USA, [3]Universtiy of Leeds, UK, [4]The Scripps Research Institute, USA, [5]University of Pittsburgh, USA, [6]University of Pittsburgh School of Medicine, USA, [7]National Institute of Health, USA, E-mail：tsuruta@slac.