and limitations of WAXS data will thus enhance both our ability to analyze WAXS experiments and their use as experimental tests of computational models of molecular systems.

Keywords: WAXS characterization, X-ray solution scattering, SAXS

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"Irena" software package for analysis and modeling of small-angle scattering data

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Availability of high-quality small-angle scattering (SAS) data is increasing with the proliferation of a wide range of high-performance user-friendly synchrotron and desktop small-angle X-ray scattering (SAXS) instruments. Similarly, neutron sources also provide an increasing number of quality and well-supported small-angle neutron scattering (SANS) instruments. As the barrier to quality data is decreasing, non-expert users - highly skilled experts in their particular fields with only limited small-angle scattering expertise - are applying the SAS techniques in their science. These users often need extensive help to be able to correctly apply the small-angle scattering methods and generate high-level science in their areas of expertise. The software package "Irena" was designed to be a comprehensive package with tools for most of the steps a user commonly needs to perform, balancing ease of use for non-expert users with the controls and complexity expert users need. "Irena" provides a number of data modeling and analysis tools, mostly applicable in such fields as materials science, polymers, and chemistry. A wide range of support tools are also included such as ones to enable input, output, manipulations with, and graphing of the data, as well as a scattering contrast calculator. As an example: one of the tools in Irena enables modeling of multiple non-interacting dilute systems with a choice of form factors and, when necessary, including one of five available structure factors. This model can be fitted to one or multiple input data sets (at once), enabling, for example, analysis of anomalous SAXS data or co-fitting of SAXS and SANS data. Other tools include "Unified fit" model, fractals model, "Debye-Bueche" model, and small-angle diffraction model.

Keywords: small-angle scattering, SAS modeling, SAS analysis

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ARP/wARP: From noisy electron densities of proteins to complete structures

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Structural interpretation of the provided experimental X-ray data, which have a low level of the information content, that therefore leads to a noisy and troublesome interpretable electron density map is a challenging task in the protein crystallography. An important carrier of the structural information in electron density maps of proteins is the repetitive chemical motif of the peptide unit that links the amino acids. One efficient way for the peptide recognition

is implemented in the chain tracing module of the ARP/wARP suite, where an advanced template matching technique is applied to the shapes of the density. However, the success of the recognition process strongly depends on the level of informational content in the electron density map. Our on-going development concerns studying the functional $p(x,y,z)$ which describes the electron density map corresponding to peptides and its relation to some distance functional $r(x,y,z)$. The connection between them can be presented as radial density functional $p(x,y,z)*r(x,y,z)$. The distribution of values of the radial density functional can then be applied to the recognition of the peptide pattern. The method is rotation invariant and its combination with the existing technique that uses the template matching improves the completeness of the protein structure provided by ARP/wARP.

Keywords: protein structure determination, electron density, pattern recognition

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Density modification by directed evolution of electron density maps

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There are numerous cases in macromolecular X-ray crystallography where current methods of density modification are not capable to yield an interpretable map. Since the performance of the automatic procedures for model building of the corresponding protein (e.g. RESOLVE, TEXTAL or ARP/wARP) strongly depends on the quality of the phases, reliable methods for modifying the density are absolutely essential. We are developing a new iterative density modification method which is based on directed evolution of the electron density map. One of the central aims for the new method is to be applicable to cases when the resolution of the data is lower than 3 Å. In a first step each grid point of the initially phased map is analysed by statistical and pattern recognition methods to define a likelihood whether the density value of the point should be changed. A small number of map points are subsequently 'mutated'. Finally, the phases from the mutated map are used to generate a new density distribution. First encouraging results with 3 Å resolution test cases have been obtained, where this iterative procedure lead to a reduction of the phase error of about $0.2°$ for each iterative step of the procedure. These will be presented and discussed. The application of the method to the crystallographic use of low resolution images from electron microscopy studies will also be presented.

Keywords: density modification, pattern recognition, protein crystallography

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Validation and correction of carbohydrate 3D structures

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Carbohydrate structures in PDB entries exhibit a rather high rate of errors [1,2]. Some errors, such as wrong residue names, surplus atoms in the glycosidic linkage, or wrong connectivities, can be