of PED patterns without full knowledge of the structure, a major step in realizing the goal of inverting PED data to obtain the underlying structure factor amplitudes.

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Keywords: precession electron diffraction, dynamical electron diffraction, electron crystallography

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High-throughput crystallization-to-structure pipeline at RIKEN SPring-8 Center

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A high-throughput crystallization-to-structure pipeline for structural genomics has been developed at Advanced Protein Crystallography Research Group (APCR-group) of RIKEN SPring-8 Center, Japan. The structure determination pipeline includes three elemental technologies for automation developed in RIKEN SPring-8 Center: the automated crystallization and observation robot system TERA; X-ray diffraction data collection using the SPring-8 Precise Automatic Cryosample Exchanger SPACE; automatic X-ray data analysis from phasing to model checking/revision using the Package of Expert Researcher's Operation Network PERON. During five years from 2002, 234 of cryoloop-mountable crystals, 175 of diffraction data sets and 149 of refined structures have been produced from 437 of purified proteins in APCR-group, by seven researchers with assistance of the developed pipeline. Used protocols in this pipeline will be introduced.

Keywords: protein crystallography, structural genomics, automation

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There and back again: Using simulated diffraction images to optimize data processing by Elves

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Modern data processing automation packages such as Elves work very well with high-quality diffraction data, but it is not surprising that Elves will fail to solve data sets that are of such poor quality that they cannot be solved manually. In between these extremes is a threshold of "solvability" that is critical to understand if we are to formulate optimal data collection strategies and robust data processing algorithms. To this end, a realistic simulation of the entire diffraction experiment (called MLFSOM) was constructed and includes most every source of error, including photon-counting noise, detector read-out noise, shutter jitter and radiation damage. The image files from this simulation were then fed into Elves and the transition between a successful structure determination and a hopeless data set was studied. These tests evaluated the impact of "scanning" individual parameters such as exposure time, crystal size, heavy atom occupancy, mosaic spread, and other experimental parameters. A central result was that the average error in the anomalous difference measurement must be less than the average anomalous signal for structure solution to succeed, but further improvement of the anomalous signal/noise ratio does not improve the structure quality significantly. It was also found that detector read-out noise has negligible impact on anomalous differences, suggesting that dividing MAD/SAD data sets over many more images is advisable to deal with radiation damage. This strategy was tried in practice and found to be superior to conventional MAD/SAD data collection.

Keywords: simulation X-ray diffraction, automatic structure solution, threshold of solvability

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Signal-based data collection: A novel approach to on-site auto-structure determination at SER-CAT

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At SER-CAT, beamline setup, sample handling, sample alignment, data collection strategy, data collection, data reduction, structure solution and data archive are on the verge of full automation. Building on these technologies a new data collection paradigm we term Signal-Based Data Collection (SBDC) is being developed aimed at increasing the success rate of structure determination and overall beamline efficiency. The SBDC approach differs from beamline automation being developed elsewhere in that it is driven by the goal of automatically collecting enough data from one (or more crystals) to ensure that the anomalous scattering signal in the final scaled data is sufficient to solve the structure. Key to our approach, and what differentiates from other developments, is that there is direct feedback from the data reduction process to the data collection process. To achieve our goal we are developing and refining an intelligent software system that allows fully automated data collection and data processing that is integrated with SER-CAT's beamline control and sample mounting systems. This database-driven expert system will monitor data collection and automatically make decisions about the data collection process based on predefined trigger values. The proposed system will also be linked to the SGXPro automated structure determination engine at SER-CAT so that users can leave the beamline with a structure in hand. Details of the implementation of various aspects of the SBDC approach will be presented. Work is supported in part with funds from SER-CAT, the Georgia Research Alliance, the National Institutes of Health (GM62407) and the University of Georgia Research Foundation.

Keywords: automated data collection, monitoring and feedback in data collection, automated on-site structure determination