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An overview of informatics developments for managing target selection to X-ray data collection

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The drive toward high throughput in structural biology has resulted in many technical innovations and developments. From ligation-independent cloning through nanolitre-scale crystallization to automated data collection the effects of these developments are changing the process of macromolecular structure determination for all laboratories, large and small, and dramatically extending our ability to address challenging scientific problems. Informatics and data management systems have also seen rapid development, and indeed for true high throughput they have become absolutely essential. Areas covered by these developments include:
- annotation of potential targets and target selection;
- construct and primer design;
- laboratory information management systems (LIMS) for tracking experimental work in the laboratory;
- managing setup and monitoring of crystallization trials;
- requesting and scheduling of resources such as synchrotron beam time;
- tracking storage and exchange of samples (such as shipping crystals to synchrotrons);
- controlling beam lines for both manual and automated data collection;
- data reduction and formulation of data collection strategies;
- techniques for automated structure solution, refinement, annotation and deposition;
- software for tracking progress of targets along the pipeline.

The Oxford Protein Production Facility (OPPF) has been at the forefront of many of the developments in Europe, and through collaborative projects such as SPINE (www.spineurope.org), eHTPX (www.e-htpx.ac.uk) and PiMS (www.pims-lims.org) it is endeavouring to make these developments relevant to other structural biology groups. This presentation provides an overview (with a European perspective) of the current state of informatics developments for the first part of this pipeline - as far as x-ray data collection - by describing the informatics techniques developed by these collaborations and regularly employed at the OPPF. Areas that will be covered in more detail include target selection, the current state of development of the PiMS LIMS, crystallization and developments toward automated/remote synchrotron data collection.

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Auto-Rickshaw: An automated crystal structure determination pipeline as an efficient tool for fast validation of an X-ray diffraction experiment

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We present an automated crystal structure determination platform, *Auto-Rickshaw* [1]. It contains several distinct computer coded decision-makers, which invoke a variety of macromolecular crystallographic programmes/programme packages during the structure determination process. A large number of structure determination paths are encoded in the system and the optimal path is selected by the decision-makers as the structure solution evolves. The primary aim of the pipeline is to validate the crystallographic experiment at the synchrotron site while the crystal is still at or near the beamline. Therefore, the system has been optimized for speed, so that typically within a few minutes, it is apparent whether or not the already collected data will be of sufficient quality to allow successful structure determination. The platform has been installed on a 16-processor Linux cluster and is remotely accessible to the beamline users via a web-server (*www.embl-hamburg.de/ Auto-Rickshaw*). An overview of the *Auto-Rickshaw* pipeline with its design, functionality, some examples and the way this platform is used as a feedback system for X-ray data collection or validation of X-ray experiment, will be discussed.

[1] Panjikar, S., Parthasarathy, V., Lamzin, V. S., Weiss, M. S. & Tucker, P. A. *Acta Cryst.* 2005, D61, 449.