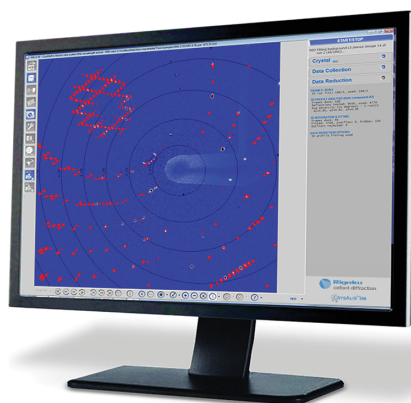


# Single crystal diffraction software

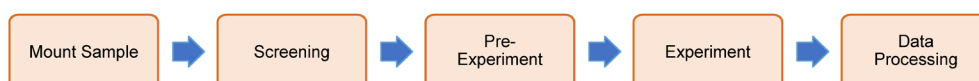


## 1. Introduction

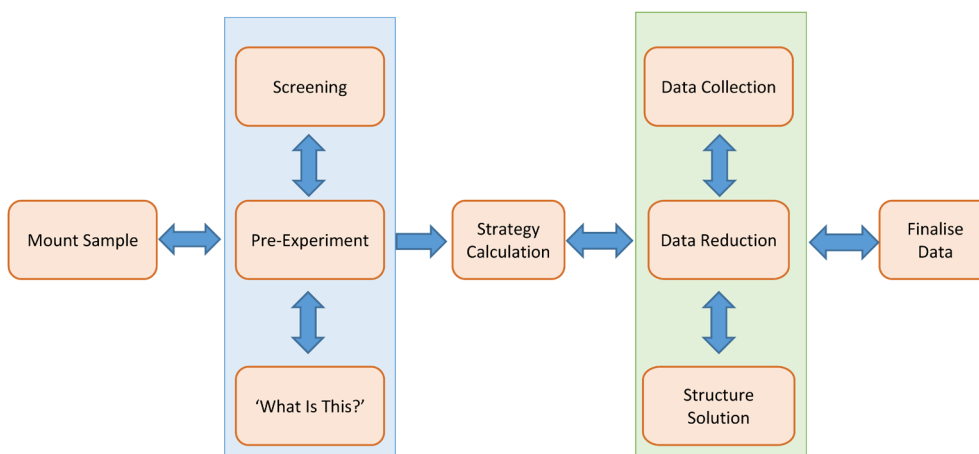
Rigaku Oxford Diffraction single's crystal diffraction systems are controlled with the user-inspired CrysAlis<sup>Pro</sup> software. CrysAlis<sup>Pro</sup> integrates and interfaces seamlessly with not only our own equipment but also with third party data collected on other diffraction systems. It delivers precise system control and superior X-ray data quality and analysis.

## 2. Software architecture

The structure or workflow of the software is key in allowing data collection to proceed in the most efficient manner without compromising quality. Traditional software architecture uses a linear path (Fig. 1) to acquire data, with other commercially available software currently requiring manual input after the end of the experiment. Using this linear method means that any



**Fig. 1** Traditional linear approach to data collection.



**Fig. 2.** The CrysAlis<sup>Pro</sup> software architecture. Arrows represent Feedback loops between the stages. Blue shaded area use 'on-the-fly' cell indexation and data analysis concurrent with data collection. Green shaded area uses 'on-the-fly' concurrent data indexing, reduction and automatic structure solution.

changes in parameters during data collection often require termination of the process and returning from the first step, which can leave unwanted, useless data on the computer hard drive.

CrysAlis<sup>Pro</sup>, however, incorporates feedback loops to teach the system, driving a more efficient pathway (Fig. 2). The scope of this software also extends beyond the data collection stage through to on-the-fly data processing and automatic structure solution. An additional, optional step called 'What is this?' (WIT) has been inserted into the process between the screening and experiment stages. The value of WIT is described in section 3.3.

This user friendly and logical workflow allows the user to screen multiple samples within one project folder, it offers various methods to screen or collect a sample data set whilst optimising parameters such as a suitable exposure time, scan width and strategy.

This workflow strategy also uses many concurrent processes to decrease the time it takes to evaluate the data. Regular feedback is supplied as to the success of the experiment during the concurrent data collection, data reduction and structure solution stages and provides

the user with alerts should any changes be required.

### 3. Key features of CrysAlis<sup>Pro</sup>

#### 3.1. Choose between SMX or PX applications

For small molecule and protein X-ray diffraction systems, CrysAlis<sup>Pro</sup> provides comprehensive crystallographic data collection and data processing in a single, fully integrated software solution.

Simply toggle between small molecule (SM) and macromolecular (PX) modes for fully optimized workflows and data reduction routines (Fig. 3). Both non-experts and crystallography specialists can set up, run and process experiments intuitively and efficiently, in fully automatic, semi-automatic and manual modes, adjusting analytical strategies for a wide variety of experimental targets including redundancy, time and resolution. An intelligent pre-experiment evaluation of crystal quality automatically suggests optimal experimental parameters, increasing productivity and accuracy. CrysAlis<sup>Pro</sup> boasts a comprehensive package of absorption correction methods and a highly effective range of specialized tools and functions for the most complex datasets. Synchrotron data can be imported, and experimental results for use in other crystallography software.

#### 3.2. Fast sample screening

With subtly different default parameters, screening for protein and chemical samples has been streamlined for each mode to allow rapid switching of samples and measuring snapshots to gauge the quality of each crystal (Fig. 4).

The goniometer drives to a convenient mounting position, which is maintained during the screening process to avoid the need to wait for the goniometer to reset, speeding up the mounting process. A clear large picture of the crystal is displayed on the monitor within the cabinet and electronically controlled dimmable lighting, both at the sample and within the cabinet surrounding cabinet, can be used to achieve the optimal video image.

#### 3.3. Unique 'What is This?' feature

Sometimes it is useful to determine the molecular structure quickly, without the need for full

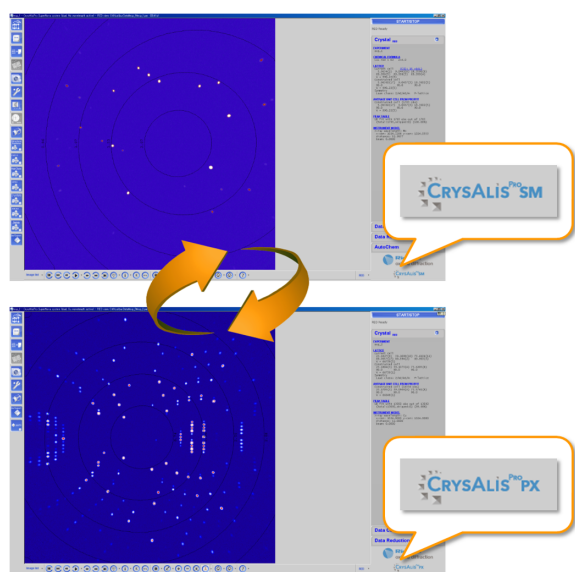


Fig. 3. Switch between SM and PX mode with the click of a button.

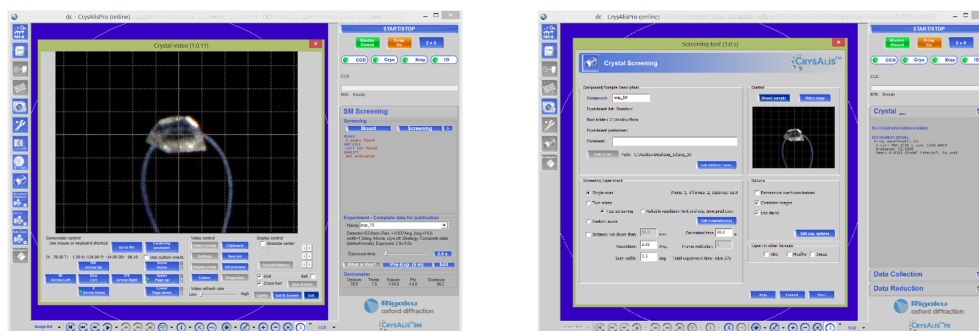


Fig. 4. Snapshots of the CrysAlis<sup>Pro</sup> screening GUI's for SM (left) and PX (right).

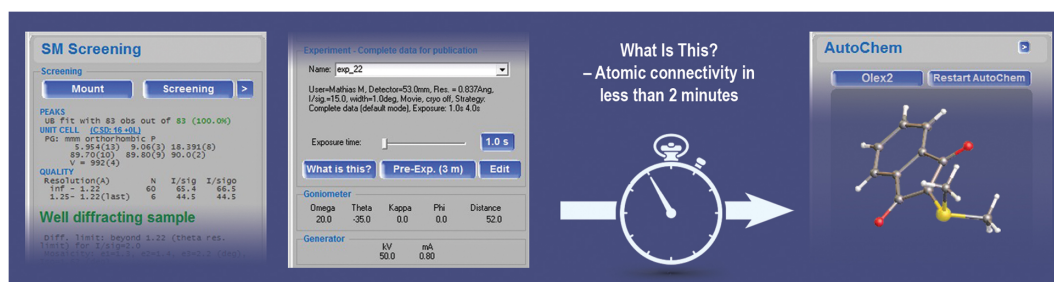


Fig. 5. The 'WIT' tool.

publishable-quality data. This is especially true in today's fast-paced research programs where molecular connectivity of intermediates in a synthetic pathway is required before moving on to the next stage. The new 'What is this?' tool is designed to provide a structure as fast as possible (Fig. 5).

Using the latest AutoChem2.1 (the automatic structure solution module) and Rigaku Oxford Diffraction's advanced hardware, it is often possible to identify a sample from a fully determined structure in under a minute. Using carefully selected strategies, the 'What is this?' tool allows for the fast collection of a minimal dataset solely aimed at providing a structure. Following sample screening the 'What is this?' tool becomes available for fast sample identification. The user may choose to continue with a traditional pre-experiment or attempt to identify the structure using 'What is this?'. The tool requires only a list of elements present in the structure and an exposure time. Using diffraction observations from the screening experiment as a basis, appropriate exposure times will be recommended by the software, although users may choose their own as desired. The list of elements is optional but recommended for the highest success rate. A solved structure is typically available within a few minutes, but can take less than a minute for strongly diffracting crystals. The symmetry and unit cell are known with more certainty when even a rudimentary structure is available, reducing the chance of erroneous data collection. Once structure factors are known, the strategy module can use them to extrapolate to target resolution for full experiments, giving better predictions of reflection intensities and thus calculated exposure times leading to higher quality efficient data collection.

### 3.4. Rapid and tuneable data collection strategies

If screening has found a candidate of interest, then the next step is data collection. The key to good data, especially with modern day four-circle kappa goniometers, is a carefully calculated data collection strategy. While the system and software provide good feedback about the sample, the user will have more insight into what parameters will achieve a quality result. This approach is facilitated by an intuitive tool that allows users to change many experiment variables to achieve the ideal dataset for your sample.

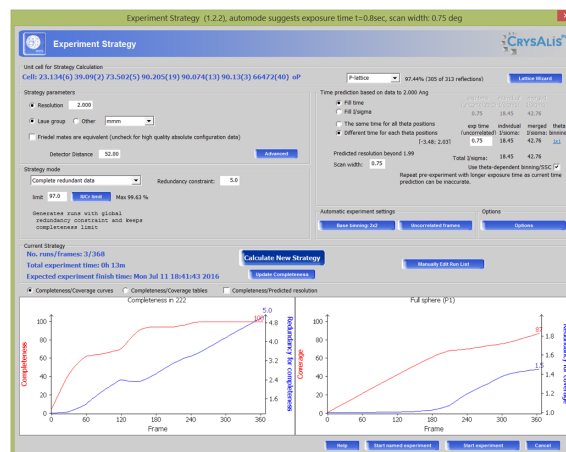


Fig. 6. Rapid strategy calculation.

The strategy prediction tools, including intensity estimation, have been thoroughly tested to ensure high accuracy (Fig. 6). This avoids the need of having to collect more data to achieve higher completeness or redundancy later. For example, small molecules that exhibit **twinning** or multi-crystals use up to four lattice orientation parameters to calculate a full strategy to collect complete data on all components. When a monoclinic cell has a beta angle close to 90°, it can appear to have orthorhombic symmetry. A simple change of Laue group will ensure that a strategy for the lower symmetry is used. Later, either during or at the end of the experiment, more data can be appended as more is learned about the structure. AutoChem is an invaluable tool for this type of situation.

### 3.5. A comprehensive range of specialist tools and solutions for the most difficult challenges

CrysAlis<sup>Pro</sup> Small Molecule offers powerful and effective specialist tools to get maximum information from experiments with non-standard or difficult crystals. It has precise controls and user-friendly **twin deconvolution tools** that can make the structure solution and refinement of twin lattices as trivial as for a standard single crystal (Fig. 7).

Other features include:

- Movie based **face-indexing** and **absorption correction**, for high-absorbing or anisotropic crystals.
- Graphical tools and data processing to identify

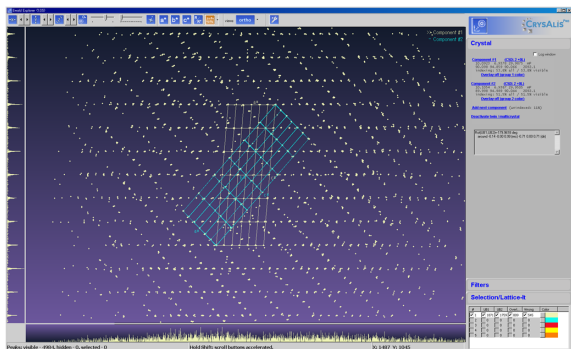


Fig. 7. Lattice Wizard for simple twin deconvolution.

and index superstructure reflections from **incommensurate structures**.

- Straightforward **multi-temperature** programming and automatic cryo-device control.
- Detailed **absorption corrections** accounting for a wide variety of challenging samples and processes.
- Generate a powder pattern from a single-crystal experiment, and collect powder patterns from polycrystalline samples.

CrysAlis<sup>Pro</sup> is equipped with the ability to collect and reduce data at high pressure following a simple procedure. A diamond anvil cell (DAC) squeezes the crystal between the faces of two diamonds. The DAC is mounted on a diffractometer and data is collected while the sample is subjected to a specific pressure. Although the DAC limits the amount of data that can be collected, CrysAlis<sup>Pro</sup> software can rapidly determine data collection strategies for these high pressure experiments. The software also automatically accounts for areas of diffraction images masked by gasket shadows during integration.

### 3.6. Obtain CrysAlis<sup>Pro</sup>

The software is freely available for users of Rigaku Oxford Diffraction equipment and can be downloaded from our forum. Register at [www.rigakuxrayforum.com](http://www.rigakuxrayforum.com).

Any queries related to the software may be answered on the forum.



QR code for the website URL of the forum

## 4. Utilizing CrysAlis<sup>Pro</sup>

This advanced software is available to both Rigaku Oxford Diffraction users and their collaborators with free multi-user, multi-site licenses. Comprehensive support and frequent updates with new, user-inspired features is offered to all users. Onsite training from expert application scientists is provided with all new system installations, giving the user everything needed to unlock the full potential of the X-ray diffractometers. User feedback to applications and software experts is actively encouraged so new and improved functionality can be added into new software releases.

