

PX Scanner

In-Situ X-ray Diffraction: Screening Proteins in the Crystallisation Plate

Data Sheet

The PX Scanner is the revolutionary product from Agilent Technologies which has been designed specifically for the identification and X-ray diffraction analysis of protein crystals in-situ within multi-well crystallisation plates.

The PX Scanner is unique in being both an optical and an X-ray imager in one compact self contained unit. The optical imaging component allows the user to visually locate and select objects which can then be studied by X-ray diffraction using the built in microfocus X-ray source, optics and CCD detector.



Figure 1. The complete PX Scanner system.



Agilent Technologies

The PX Scanner is the ideal system for applications in:

Crystallisation Screening

- Identify crystalline matter
- Discriminate salt from protein
- Identify optimum conditions

Crystal Selection

- Quantify crystal diffraction properties
- Identify the best crystals in the well



Figure 2. Inserting a crystallisation plate into the PX Scanner.

Experimental

An SBS format plate is inserted into the PX Scanner, and an optical scan of each well with automatic focus is carried out. The optical imaging process automatically stores a picture of each sample well with the control software allowing images to be reviewed during the acquisition and crystals placed in a prioritised queue for X-ray diffraction analysis. The software maintains a database of all collected images and X-ray diffraction analyses for recall at anytime in the future.

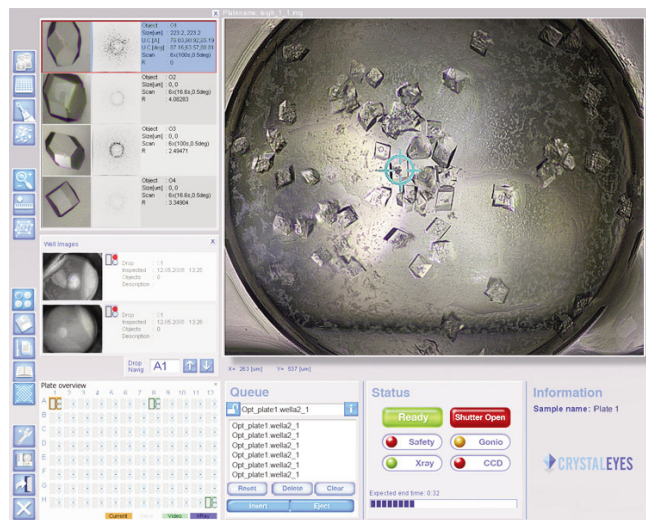


Figure 3. PX Scanner control software.

Intelligent Background Subtraction and Unit Cell Finding

Figure 4 shows a six degree scan of a thaumatin crystal growing in-situ in a 96-well crystallisation plate. Background scatter from the plastic and drop solution can be clearly seen as a circular ring peaking at around 5–6 Å. The PX Scanner software applies background removal algorithms to remove this noise and allows peak hunting and auto indexing of the unit cell; in the case tetragonal $a = 58.657(5)$ Å, $c = 151.63(3)$ Å.

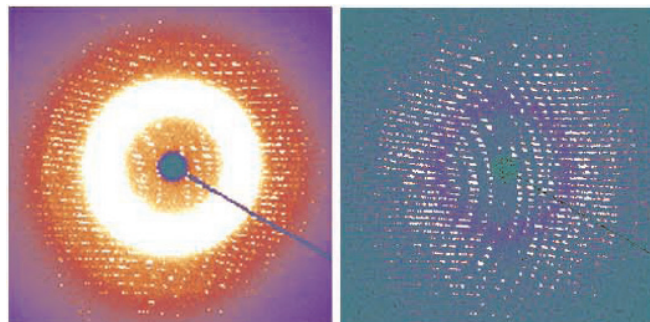
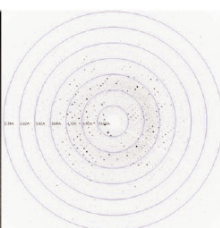
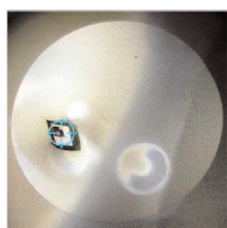
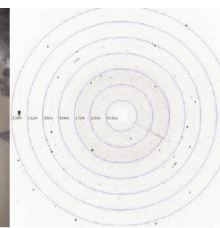
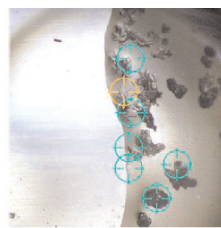


Figure 4. Background subtraction. Left: original image; right: background subtracted.

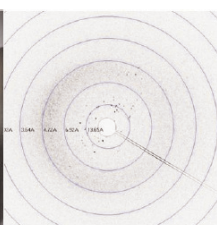
Discrimination of Salt From Protein Crystals



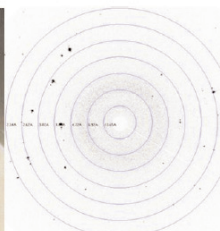
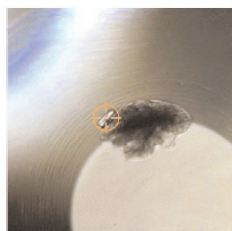
Good diffraction to 2.3Å:
Protein



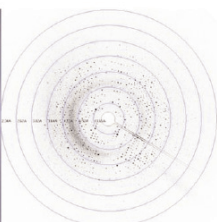
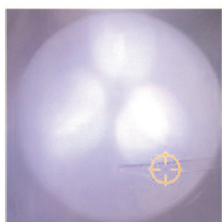
High-angle diffraction:
Salt



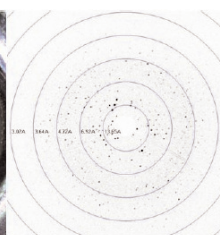
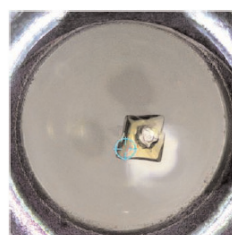
Weak low-angle diffraction to 4Å:
Protein



Strong high-angle diffraction:
Salt



Good diffraction to 2.5Å:
Protein



Strong but disordered diffraction to 3.0Å:
Multiple protein crystal

⊕ Indicates actual crystal, or group of crystals X-rayed.

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