



Agilent SuperNova and PX Scanner Systems

COMPACT, HIGH-PERFORMANCE SOLUTIONS FOR STRUCTURAL BIOLOGY

The Measure of Confidence



Agilent Technologies

COMPACT, HIGH-PERFORMANCE SOLUTIONS FOR STRUCTURAL BIOLOGY

Fully-integrated and cost-effective systems for in-house protein crystal screening and data collection, with user-friendly workflows for multiple users and maximum efficiency.

The Agilent SuperNova and PX Scanner systems provide a range of unique capabilities and benefits to meet the needs of modern structural biology facilities. From crystallization screening to full data collection, our compact, cost-effective and user-friendly systems offer the ideal in-house solution to complement visits to synchrotron beamlines.

The increasing number of synchrotron facilities has resulted in a dramatic decline in the use of traditional large, high flux – and high maintenance – rotating anode generators in protein crystallography laboratories. High beam flux is no longer the main factor when assessing the latest systems, with high reliability, low maintenance and overall cost of ownership now all equally important. The turnkey nature of sealed-tube micro-focus systems offers high performance and maximum uptime, all at an affordable price.



The compact PX Scanner and SuperNova systems installed side-by-side in a structural biology laboratory.

USER-FRIENDLY CRYSTAL SCREENING WORKFLOW

Designed to make crystal screening as effortless as possible, the PX Scanner – combined with Agilent’s CrystalEyes software platform – offers an efficient and non-destructive alternative to traditional crystal screening techniques.

The PX Scanner is Agilent’s unique instrument dedicated to the *in-situ* screening of protein crystals in multi-well crystallization plates.

Combining optical and X-ray imaging in a single compact instrument, the PX Scanner facilitates visualization, identification and X-ray evaluation of protein crystals undisturbed within the growth media.

An unlimited number of crystals can be queued for X-ray analysis, either within one well or over an entire plate. The PX Scanner then automatically processes the queue, leaving the user free to continue with other work before reviewing the diffraction results.

By removing the need for manual handling of crystals during screening, the PX Scanner can accelerate the process of obtaining suitable crystal samples at all stages of the crystallization workflow, including:

- High throughput crystallization condition screening
- Crystallization scale-up for diffraction quality crystals

Benefits of the PX Scanner

- Early stage identification of crystalline material
- Differentiation of salt from protein crystals
- Identification of optimal crystal growth conditions
- Comparison of crystal diffraction quality
- Automated crystal screening leading to accelerated results
- Study of crystals too fragile to extract
- Optimization of harvesting and cryo-protectant solutions



Inserting a multi-well crystallization plate into the PX Scanner.

AGILENT PX SCANNER CRYSTAL SCREENING SYSTEM



The PX Scanner is fully self-contained, with a modular construction.

View Inside the PX Scanner

System modules from top to bottom:

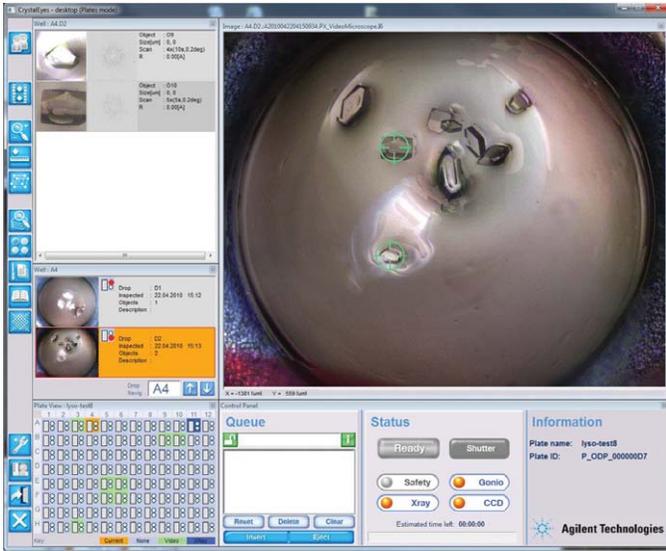
- X-ray safety panel
- System interface
- System computer
- X-ray generator
- X-ray source/CCD detector chiller

Features

- Vertically-mounted 2nd generation micro-focus Nova X-ray source
- 135 mm active area CCD detector
- Touch-screen control and barcode reader for plate identification
- Up to 6° plate tilt
- Accepts virtually all SBS-format plates
- Ultra compact — system footprint < 1 m²
- Total power consumption < 1 kW
- CrystalEyes — user-friendly software for all optical and X-ray screening plus secure data storage

PX Scanner Applications





The PX Scanner has a barcode reader for plate identification and plates are inserted using touchscreen control. Optical and X-ray screening experiments are carried out and logged using Agilent's user-friendly CrystalEyes software platform.

X-ray Imaging

Housed within the base of the system the high intensity Nova X-ray source is orientated to provide a vertical X-ray beam. After optical imaging of the droplets and selection of potential crystals for *in-situ* X-ray analysis, the plate and crystals in turn are accurately and automatically positioned directly over the X-ray beam, which travels vertically up through the horizontal plate and crystal. The plate and thereby crystal can be tilted up to 6°, allowing scanned X-ray images to be collected. The diffraction data are automatically recorded above the plate by an Agilent 135 mm CCD detector.

Plate Compatibility

Highly versatile, the PX Scanner accepts virtually all crystallization plates, micro-fluidic chips and counter-diffusion set-ups which fully conform to SBS format.

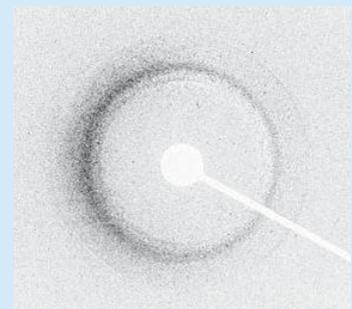
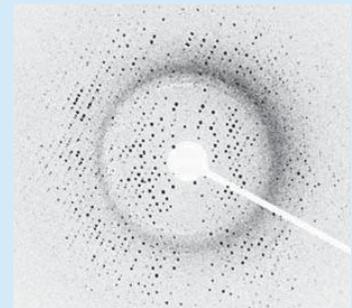
More Sensitive than Ever

The PX Scanner now incorporates the second generation Nova X-ray source for maximum sealed-tube X-ray intensity. Combined with a more sensitive CCD detector, the PX Scanner's unique ability to efficiently screen crystals is more powerful than ever before.

The Agilent PX Scanner Crystal Challenge

Two protein crystals grow in the same drop in a multi-well crystallization plate. One diffracts, the other does not. You have only one chance of success, as disturbing the drop means the second crystal dies. Which one would you choose?

How good are you at screening crystals by eye? Find out at www.agilent.com/lifesciences/crystalchallenge.



SEALED-TUBE SIMPLICITY FOR IN-HOUSE PROTEIN CRYSTALLOGRAPHY

The Agilent SuperNova is the ideal system for in-house data collection, combining a high brilliance sealed-tube micro-focus X-ray source with high sensitivity CCD detector in a compact, fully integrated platform.



Mounting a crystal on the SuperNova.

Compact and Self-contained

At less than 1 m², the SuperNova has the most compact footprint of any modern research-grade diffractometer. The system is entirely self-contained within a safety-interlocked radiation protection enclosure, is compliant with all local safety directives and is powered through a standard electricity supply.

Housed inside the cabinet, behind a radiation protection window, the X-ray source, goniometer and CCD detector are illuminated by cool LED lighting, which can be controlled through both hardware and software.

Easy Sample Mounting

Sample mounting and alignment on the SuperNova are quick and easy using a dedicated color video microscope with 120x magnification. Sample illumination is provided by focusing LEDs mounted on both sides of the system beam stop. A software-enabled sample alignment assistant is also available in CrysAlis^{Pro}.

Where greater access is required for mounting crystals with cryotools, the SuperNova's beam stop assembly can be rotated out of the X-ray beam path and the CCD detector automatically driven away from the sample position.

Modular Design

Designed with ease of service and support in mind, the SuperNova has a modular construction with each major component being a self-contained and easily exchangeable unit. Contained within the base of the SuperNova these units include:

- System control interface
- Multi-core computer
- X-ray generator
- X-ray generator chiller
- CCD detector chiller

Multi-Core Computer

The SuperNova's computer handles everything including automatic data collection, rapid multi-core data processing and structure determination. Within the software, the machine control is separated from the crystallographic applications. As such, an optional second networked PC may be added for offline processing, remote access and experimental control of the system.



SuperNova system with the optional AirCooler radiator.

Integrated X-ray and CCD Cooling

The SuperNova's X-ray source and CCD detector are cooled by built-in compact re-circulating water chillers using Peltier cooling. Water cooling provides for ultra-precise temperature control of both the X-ray source and CCD detector, independent of lab temperature, humidity or any other external factors.

The integrated chillers can be connected to a suitable external water supply or to the optional AirCooler radiator unit; making the SuperNova an entirely self-contained, air-cooled and eco-friendly system requiring only mains electricity (100 - 240 V).

Stay in Touch with Your System

Agilent's CrysAlis^{Pro} software sends user-defined system hardware and experiment status reports to a nominated email address. Full control of the system is then available by accessing CrysAlis^{Pro} using standard remote desktop applications.

Optional Cryo-devices

With a very open geometry, the SuperNova's goniometer has been designed to accept all major open flow cryogenic sample environment devices including;

- Oxford Instruments' Cryojets
- Cryostream, Cobra and Desktop Cooler devices from Oxford Cryosystems
- Agilent's liquid helium device, the Helijet (< 15-75 K)



Inside the cabinet is a 4-circle goniometer with Nova micro-focus copper X-ray source and high sensitivity CCD detector (the Titan is shown here).

SuperNova Applications

Crystal screening	Molecular replacement	Ligand binding	SAD/Heavy atom phasing	RNA/DNA	Small molecules

COMBINING THE BRIGHTEST SEALED-TUBE COPPER X-RAY SOURCE WITH SUPERIOR CCD DETECTIVITY

Agilent designs systems as complete units and manufactures all main components. With copper micro-focus X-ray sources in production since 2005 and CCD detectors since 1992, Agilent's expertise offers proven performance and reliability.

Nova X-ray Source

The SuperNova has been designed around Agilent's high brilliance Nova micro-focus X-ray source. This combines the latest in micro-focus X-ray tube technology with specially designed multi-layer X-ray optics. The orthogonal, double bounce design enables these multi-layer optics to achieve efficient capture and focusing of X-rays into a high purity and well shaped beam.

The second-generation Nova is currently the brightest copper micro-focus X-ray source available, providing data quality comparable to modern micro-focus rotating anodes.

The Nova is a low power (up to 50W) source which along with the entire SuperNova system requires only standard mains electricity. The sealed-tube configuration is highly cost-effective, requiring no routine maintenance, and is extremely simple to service when tube changes are required.



High intensity Nova micro-focus X-ray source.

Nova Source Features

- Copper wavelength
- Up to 50 W power consumption
- Low divergence
- 2nd generation – our brightest ever micro-focus X-ray source
- Proprietary multi-layer X-ray optics
- ~ 140 micron beam size
- 3-year warranty available

Second-generation: Benefits

- Measure samples you could never measure before with a sealed-tube source
- Double the diffracted intensity compared to first generation sources
- Data quality comparable to modern micro-focus rotating anodes
- Straightforward onsite upgrade available for first-generation Nova sources

CCD Detectors

A number of area detector technologies are available for single-crystal X-ray diffraction; offering a wide range of features and specifications. However, the best measure of a detector's sensitivity is the signal-to-noise ratio (SNR) of observed data. Modern detectors can correct for many inconsistencies and irregularities, but the massaging of data in software is never a substitute for good observed data. The best detectors are able to maximize SNR for both strong and weak signals over the whole dynamic range.

Maximizing Signal-to-Noise

Detector gain amplifies both signal and noise, so a high gain is of little value in a noisy detector (see images below right — the APS CMOS detector has a ~2-fold gain but an order of magnitude higher noise, resulting in less than optimum performance).

Agilent CCD detectors are built around low noise CCD chips and are optimized with very low noise electronics, providing higher signal-to-noise ratios for observed data.

Other Factors

- Speed – 4-port chip technology makes for rapid image-to-image readout times as low as 0.28 seconds
- Dynamic range – $\geq 50,000$, equal to or higher than any other CCD detector
- Tuneable spatial resolution – optimized binning modes (4x4 for ultimate sensitivity, 1x1 for ultimate resolution)
- CCD chips – high linearity ($< 1\%$ deviation) and no tiling, therefore no gaps between chips
- Proven reliability – confidence in our CCD technology is matched by a warranty of up to 5 years



Atlas

The optimum combination of large active area ($\text{\O}135\text{ mm}$) and detector sensitivity, the Atlas is the ideal choice for fast, high quality data collection.

- Truesense Imaging KAF4320 CCD chip
- Active area $\text{\O}135\text{ mm}$
- Speed, 0.28 s (duty cycle)
- Gain, $90\text{ e}^-/\text{X-ray (Cu)}$
- Precision, 18 bit (hard wired)
- Low noise



Titan

The largest detector in the Agilent range ($\text{\O}165\text{ mm}$). The Titan collects more data per image than any other large active area CCD detector.

- Truesense Imaging KAF4320 CCD chip
- Active area $\text{\O}165\text{ mm}$
- Speed, 0.28 s (duty cycle)
- Gain, $24\text{ e}^-/\text{X-ray (Cu)}$
- Precision, 18 bit (hard wired)
- Low noise

Agilent Atlas CCD



APS CMOS (Agilent R&D)



Comparison of the observed signal from an Agilent Atlas CCD detector and an APS CMOS detector (developed by Agilent's X-ray diffraction R&D group). Both images are taken through an identical grating, using 5 second exposure times. Despite the CMOS detector having a higher gain, the much stronger-looking image on the left demonstrates the greater signal-to-noise ratio (SNR) the Atlas CCD provides.

USER-INSPIRED SOFTWARE FOR SUPERIOR DATA QUALITY

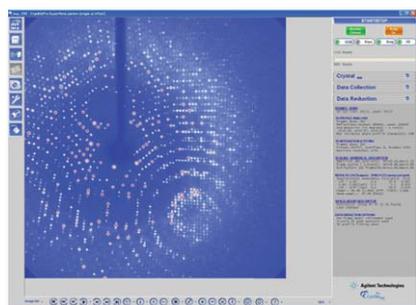
CrysAlis^{PRO} PX is Agilent's user-inspired data collection and data processing software for protein crystallography. Designed with an easy-to-use interface, CrysAlis^{PRO} PX can be operated automatically, semi-automatically, or manually.

Automated Crystal Screening

At the heart of CrysAlis^{PRO} are automatic crystal screening, data collection and data reduction features. A user-friendly crystal screening mode allows for quick and efficient screening of multiple crystals in succession, automatically providing unit cell parameters, I/sig values and effective diffraction limits for each crystal. Full data collection can then be carried out with a single click.

Fastest Strategy Software

CrysAlis^{PRO}'s sophisticated strategy software automatically calculates the optimal conditions for fast, high quality, complete data collection based on the unit cell and diffraction power determined in the screening experiment. Minimal user interaction is required, although the experiment parameters can be manually determined if desired.



Main CrysAlis^{PRO} PX GUI.

Automatic and Concurrent Data Reduction

Data reduction and processing initialize automatically with the start of data collection and employ intelligent routines which tune the parameters to give the best data quality. Processed data are always available and accompanied by real time on-screen feedback of data quality and completeness. CrysAlis^{PRO} is programmed for multi-core data processing, meaning rapid results even from the largest data sets.

CrysAlis^{PRO} PX has a quick link to the CCP4 software suite (where installed) and also includes a simple export feature: this outputs data in a variety of formats for use in third-party data reduction packages such as MOSFLM, DENZO and XDS.

A Full Complement of Crystallographic Tools

CrysAlis^{PRO} PX provides a comprehensive range of highly effective tools and functions for dealing with both routine and problematic data. These tools can be set automatically, or can be accessed via the user-friendly GUI or command line interface.

Hardware and Software Compatibility

CrysAlis^{PRO} seamlessly interfaces with third-party cryo-devices enabling full control in both routine and multi-temperature experiments.

While the software is principally designed for working with Agilent X-ray systems and data, it can also be used for processing data from many third-party systems and detectors. This feature is particularly useful for working with synchrotron data.

Software Updates and Licensing

The Agilent X-ray software team welcomes user feedback: CrysAlis^{PRO} is frequently updated with new features inspired by our users. In this way, our software is continually improving so that your system always provides data of the highest quality.

- CrysAlis^{PRO}, along with all future updates, is provided **free-of-charge** to Agilent system users and comes with a multi-user, multi-site license.

CrysAlis^{PRO} PX Features

- Quick crystal screening mode
- Rapid data collection strategy calculation
- Fast and concurrent data reduction
- Data collection and data reduction fully optimized for protein datasets
- Ewald^{PRO} — reciprocal lattice viewer
- Import synchrotron data, and export data for use in other programs
- One-click switch to CrysAlis^{PRO} SM for small molecule samples

CrystalEyes PX Scanner Software

Easy to Use, Graphical Interface

CrystalEyes can be used online to control the PX Scanner or offline for the review of previously recorded data. The easy to use graphical interface uses a schematic of the crystallization plate for user-selected drops of interest. Dependent upon the type of plate, one or more drops are displayed, together with a list of all data recorded, be it optical or X-ray. The user can then select any part of this data for display as a large image within the interface.

Optical Imaging

Using CrystalEyes, the PX Scanner can optically image either the entire plate or individual user selected wells / drops. All tasks are added to an on-screen queue allowing the PX Scanner to be used either in real time manual mode or unattended automatic mode.

Mouse Selection of Objects for X-ray

While reviewing optical images, objects for *in-situ* X-ray analysis are easily selected by simply clicking on the object using the mouse cursor. The software automatically queues the task, centers the crystal on the X-ray beam and collects data.

Once recorded, X-ray images can be analysed within CrystalEyes to provide information on:

- Crystal composition (salt/protein)
- Resolution limit of diffraction
- Possible unit cell parameters
- Overall diffraction quality

Secure Login and Data Storage

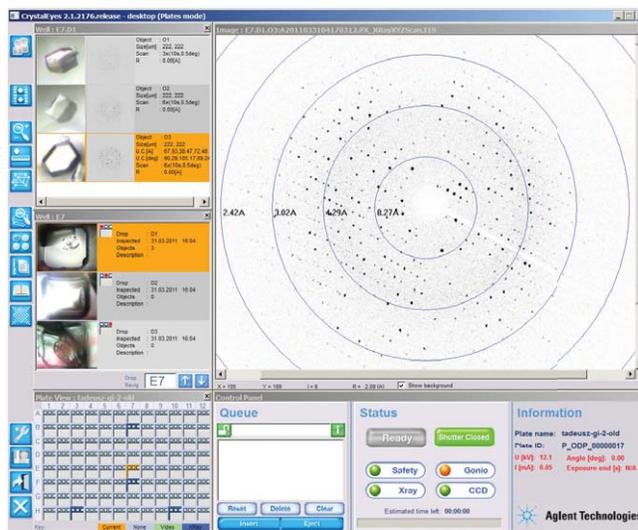
CrystalEyes operates a sophisticated, custom database which uses secure user login to control access to personal and group data.

Ease of Export of Results

All results from CrystalEyes can be exported as a concise html report with more in depth crystallographic analysis available using Agilent's CrysAlis^{Pro} software.



CrystalEyes in plate view, with a crystal targeted.



CrystalEyes with the observed diffraction image.

Learn more

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