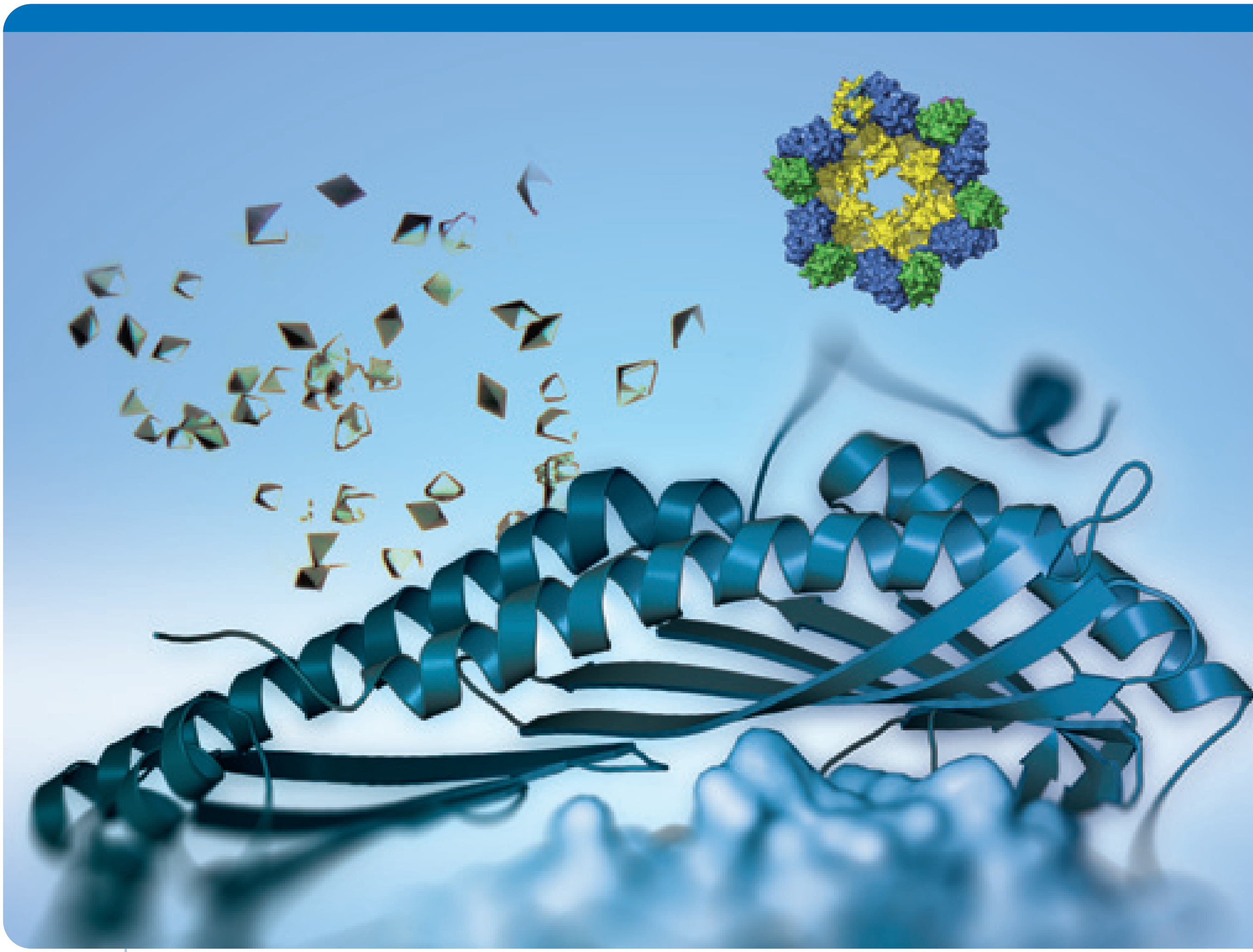


D8 VENTURE
D8 QUEST

- D8 Structural Biology Solutions

Innovation with Integrity

Crystallography

Stable and easy-to-align beam path

LED enclosure illumination

Low-temperature device options

PHOTON II™ CPAD detector

Microfocus TXS™ source

Wide doors for optimal access

METALJET™, the most intense home source

Third-generation IµS 3.0™ microfocus source


D8 VENTURE
D8 QUEST

X-ray Crystallography: Driving the Structural Biology Revolution

The field of structural biology continues to advance dramatically with researchers tackling ever more complex and challenging macromolecular structures. X-ray crystallography is a crucial tool in this ongoing quest, accounting for over 93% of the structures deposited in the Protein Data Bank in 2015.

The best in-house X-ray system can offer a significant advantage in this highly competitive field. With the latest source and detector technology, one need no longer wait for synchrotron-quality structures.

Great research deserves great tools.

Groundbreaking research is often driven by the development of improved tools. This is evident at synchrotron facilities, where the introduction of microfocus beams, faster photon-counting detectors, data-processing pipelines, and multi-axis goniometers have revolutionized data collection.

Bringing these same powerful tools to the home lab is Bruker's driving vision for the new D8 Structural Biology Solutions.

A state-of-the-art home laboratory system can contribute significantly to structural biology's quest for capability, productivity, and efficiency. A home lab system allows samples to be pre-screened before synchrotron visits—for the best use of valuable beamline time. Moreover, it is now possible to produce, in a few hours, data competitive with top synchrotron beamlines in terms of both quality and resolution.

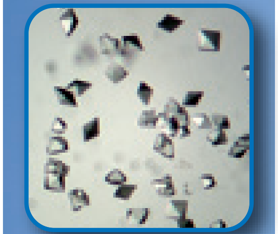
D8 QUEST and D8 VENTURE: designed with scientists in mind.

The D8 Structural Biology Solutions offer the highest standards of quality, performance, and reliability. Our designs excite tomorrow's research.

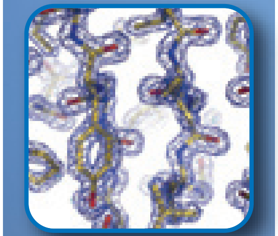
D8 Structural Biology Solutions!

Metalloproteins 1)

Microcrystals 2)

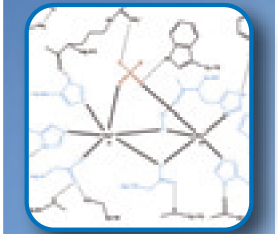


SAD phasing 3)

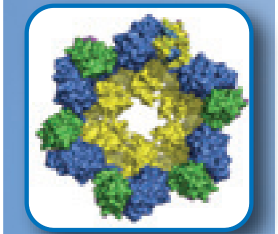


Protein-DNA complexes 4)

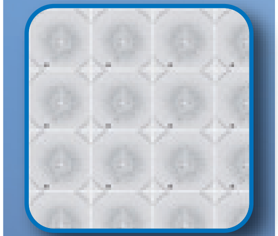
Substrate binding 5)



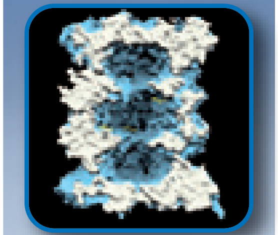
Multi-protein complexes 6)



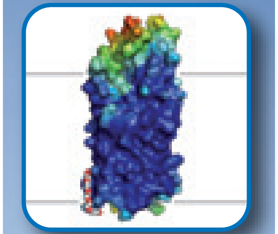
High-throughput screening 7)



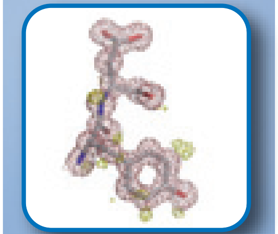
Long unit cell axes 8)



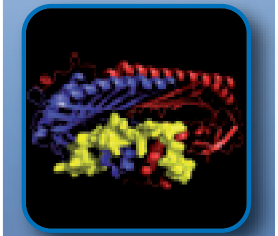
Membrane proteins 9)



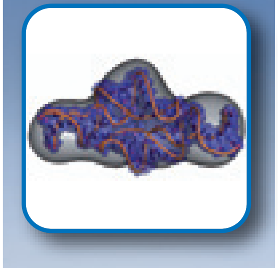
High-resolution structures 10)



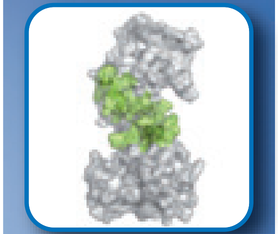
Molecular motors 11)



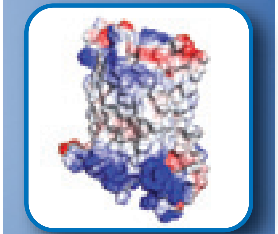
BioSAXS 12)



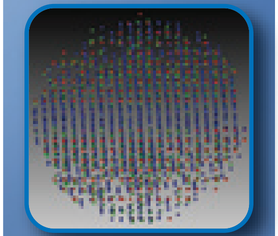
Molecular replacement 13)



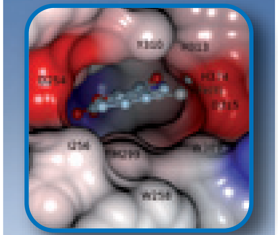
GPCR crystallography 14)



Twinned crystals 15)



Structural enzymology 16)



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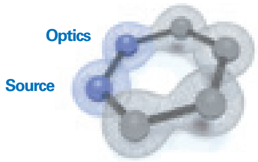



Liquid metal METALJET
with HELIOS MX optics

Brighten Up your Home Lab: METALJET, TXS, and IµS 3.0— all with HELIOS MX

High flux, stability, small beam size, and low divergence are essential for collecting the highest-quality data from challenging crystals. These requirements have driven developments in synchrotron design. Now, Bruker has applied these important lessons to home-lab source technology.

Our sources now deliver beam intensities comparable to those of typical bending-magnet beamlines. The modern METALJET now crosses the next boundary, matching diffraction limits previously only seen at third-generation synchrotrons.

These solutions combine high intensity and superior beam profiles with unmatched beam stability. Instant instrument access makes home-lab crystallography with Bruker solutions more productive than ever before.


Compact TURBO X-RAY SOURCE (TXS)
with HELIOS MX optics

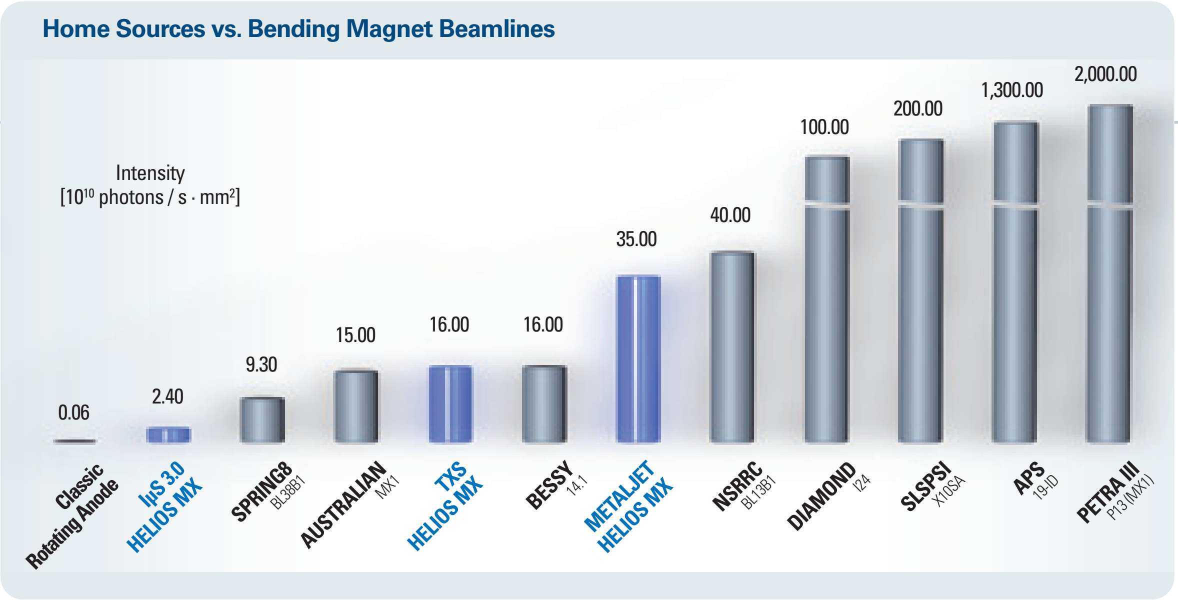
Copper is king.

Copper radiation (1.54 Å) is the most popular wavelength for macromolecular crystallography in the home lab. X-rays at this wavelength, provided by our TXS and IµS 3.0, are diffracted very strongly by the light atoms in biological molecules. At Cu radiation's wavelength, sulfur and other common scatterers also provide the anomalous signal for in-house SAD phasing.


IµS 3.0 X-ray source
with HELIOS MX optics

Gallium: the better copper.

The gallium-Kα emission line (1.34 Å) is near that of Cu for maintaining the proven benefits of Cu-Kα radiation. Yet, gallium's shorter wavelength adds a number of advantages, such as reduced radiation damage,



Home Sources vs. Bending Magnet Beamlines

increased data collection efficiency, reduced X-ray absorption by the sample, and reduced scattering by both mother liquor and air. The METALJET's ultra-intense Ga-Kα beam takes advantage of all these benefits.

Your personal beamline.

In the past, finding the right X-ray source for your lab demanded a choice between the highest performance and the lowest maintenance.

Now you can have it all: Bruker's new X-ray sources are designed to combine superb performance with unprecedented stability, maximum uptime, and easy maintenance. All of our compact X-ray sources are directly mounted on the goniometer. This ensures easy and stable downstream alignment of the source to the goniometer—greatly improving overall system precision and minimizing service efforts. All generators are fully contained within the cabinet, resulting in very compact systems with minimal footprints.

The new IµS 3.0: now with even more maintenance-free photons.

With over 750 systems installed in the 10 years since its introduction, the air-cooled IµS has developed a formidable reputation as the most reliable low-power microfocus X-ray source available, generating an impressively intense X-ray beam. The latest-generation IµS 3.0 not only delivers twice the brightness of competing sources, it also requires no routine maintenance—reducing ownership costs to near zero.

The new IµS 3.0 is the first microfocus source developed completely and specifically for crystallography, achieving higher intensity than any other microfocus source. In fact, the output of the IµS 3.0 is extremely competitive even with typical rotating anodes: over 70% of the average output with a modern microfocus rotating anode, but essentially no maintenance costs or downtime.

We are so confident of the IµS 3.0's quality that we support every one with a three-year warranty which guarantees the full specified intensity for the whole period. Others don't.

The TURBO X-RAY SOURCE: high performance. Easy living.

The TXS combines the highest performance available from a rotating anode with unprecedented ease of use. The source features a modern direct-drive anode and a vacuum chamber with integral turbomolecular pump for faster startups. Pre-aligned and pre-crystallized filament cassettes are easily exchanged in almost no time. Extended anode and filament lifetimes ensure the longest uptimes and maximum productivity.

METALJET: the X-ray revolution without rotation.

The METALJET uses a high-speed jet of liquid metal that accepts a much higher power load than the solid target of rotating anodes. This breakthrough in X-ray source technology delivers an X-ray beam an order of magnitude brighter than that achieved with traditional rotating anode sources.

With the metal jet continuously supplying fresh target material, the source intensity remains constant over time, in contrast to rotating anodes that degrade in intensity quickly due to anode roughening. Like the IµS 3.0, the METALJET is operated with single-phase power and also requires no external cooling, minimizing installation requirements.

The new METALJET now also offers dual-port operation with no compromise in performance: all new METALJETs are shipped dual-port ready. This means that you can add a system on the second port now or at any time in the future.

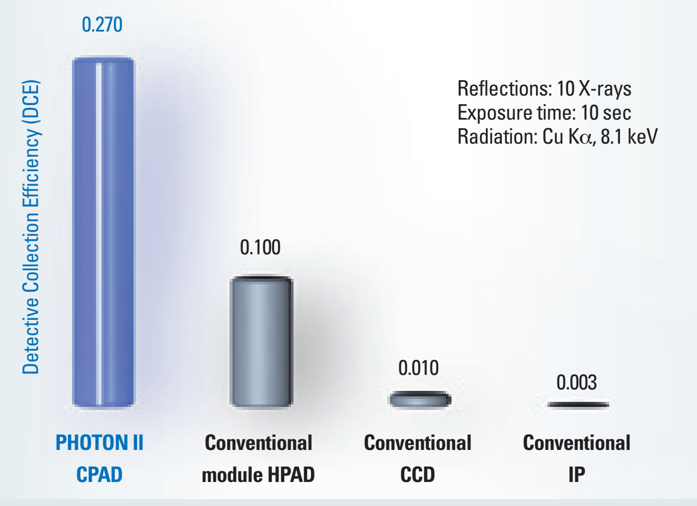
HELIOS MX: the brightest optics under the sun.

The HELIOS MX multilayer optic delivers up to three times the intensity of conventional multilayer optics. Improved deposition technology yields higher precision and greatly enhances the optics' reflectivity. For the METALJET, we specifically developed a unique low-figure-error optic. This patented optic is the only X-ray mirror that fully preserves the inherent brilliance of the METALJET. Conversely, the relatively high-figure error of other multilayer optics with the METALJET typically leads to a loss of brilliance of up to 70%.

The highly-monochromatic X-ray beam can be easily optimized to match the characteristics of each sample with a set of collimators that control beam size and divergence.

PHOTON II: The Future of Detection is Now

Detective Collection Efficiency (DCE) for various detectors



Every photon diffracted from your sample provides a quantum of information that describes the protein's unique structure. This is why the ideal detector must faithfully record each and every photon in order to preserve this precious information. The new PHOTON II detector comes very close to this ideal, with speed, sensitivity, and accuracy superior to that of any other detector.

HPAD: Hybrid Pixel Array Detectors were fast, but…

Hybrid Pixel Array Detectors (HPAD) were first introduced almost 15 years ago at third generation synchrotron sources. These first-generation pixel array detectors feature high speed, but they are far from perfect as they simply do not record every photon. Indeed, a large fraction of the incident photons are typically lost by HPADs due to several significant shortcomings:

- Small active area: laboratory versions typically only have two or three modules, wasting a large fraction of the diffracted X-rays which simply miss the detector.
- Gaps in the detector: several small hybrid sensors need to be combined to create larger detectors.
- Significant dead areas surrounding each and every pixel caused by the charge sharing effect: up to 30% of each HPAD pixel typically shows no sensitivity to X-rays.
- Typical HPADs only detect about 70% of Cu X-rays which are incident on the detector when combining all sources of signal loss including readout dead time, charge sharing losses, and gaps.

CPAD—Charge-Integrating Pixel Array Detectors: from the XFEL to your home laboratory.

To overcome the shortcomings of HPADs, a new technology—the Charge-Integrating Pixel Array Detector (CPAD)—has recently been developed for use at fourth-generation X-ray Free Electron Laser (XFEL) sources. CPADs come much closer to an ideal detector than any other technology.

The PHOTON II CPAD is the first detector to bring this groundbreaking new technology to the home laboratory.

The PHOTON II CPAD features:

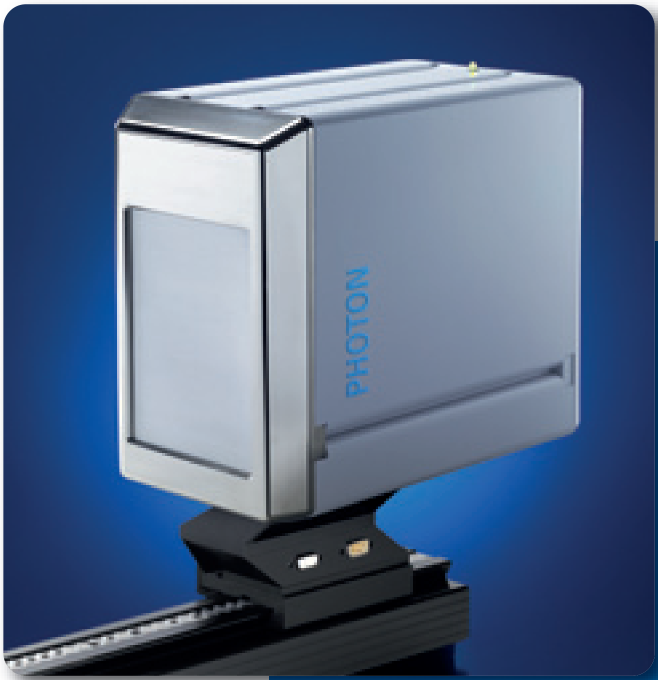
- The largest monolithic active area of any pixel array detector
- No gaps due to the use of a single wafer-scale silicon sensor
- Single-photon sensitivity
- No charge sharing effects
- Zero counting losses

The PHOTON II is up to three times larger than the laboratory versions of HPAD detectors. This means that the PHOTON II collects data much more efficiently, achieving higher redundancy and better data in less time.

The PHOTON II also features very high-speed operation at 70 frames per second, up to three times faster than conventional laboratory HPADs. This allows super-fine slicing in shutterless mode.

The bottom line: the PHOTON II produces superb data, faster than ever before possible.

PHOTON II—the future is now!



PHOTON II detector, air-cooled

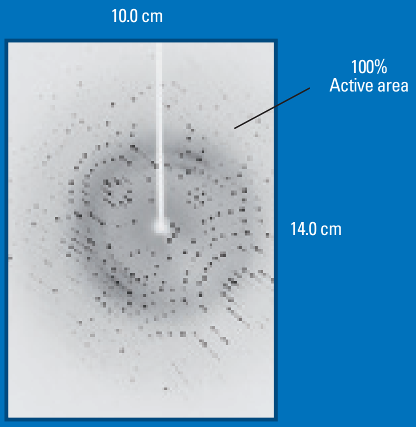
CPAD sensor, 140 cm^2

Superior PHOTON II CPAD
Charge-Integrating Pixel Array Detector

10.0 × 14.0 cm = 140.0 cm^2 active area

All Aces = High Speed, High Dynamic Range, Best Data

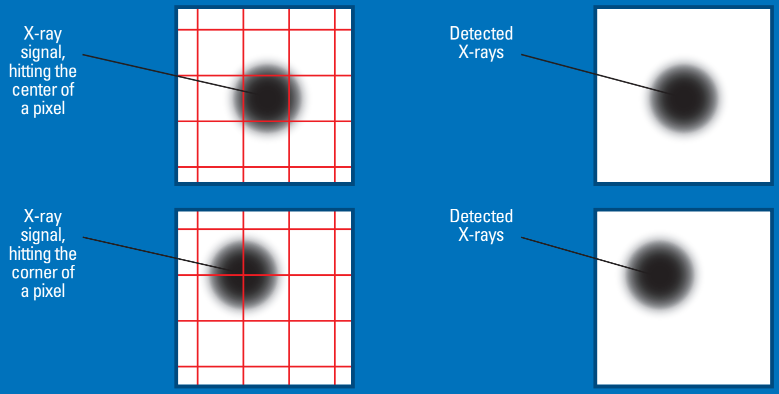
Large active area: see more from your sample, lose the gaps



The PHOTON II features the largest monolithic X-ray sensor available for superior coverage with absolutely no gaps.

No charge sharing noise: eliminate the dead border area

Incident spot → **Detected X-rays**

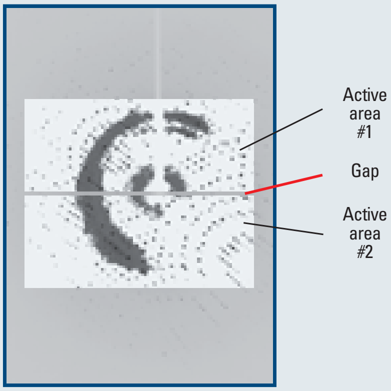


The PHOTON II has no charge sharing losses and thus no dead border areas.

Every X-ray is detected; no photons are lost.

Conventional HPAD
Hybrid Pixel Array Detector

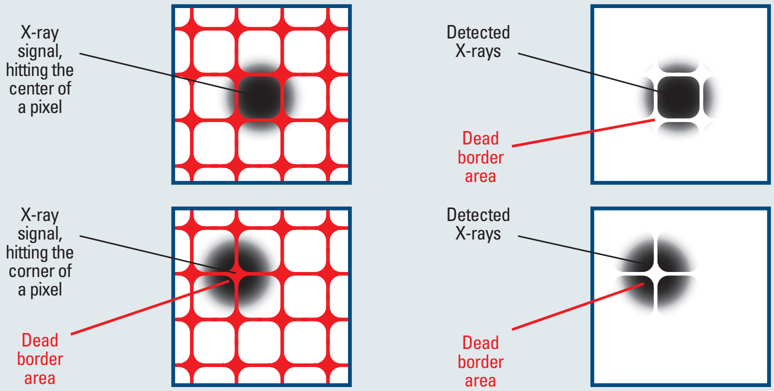
Small active area



Conventional HPADs offer relatively modest active areas and suffer from inactive gaps.

Charge sharing noise

Incident spot → **Detected X-rays**



Conventional HPADs exhibit a dead border area around each pixel due to charge sharing; X-rays hitting this dead border area are lost.

X-rays which hit the dead border area are lost, leading to “gaps” in the detected reflection.

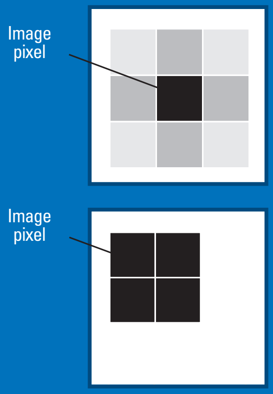
Best Linearity
Large Active Area
Best Spatial Resolution
Detect All X-rays

Detector

PHOTON II holds All the Aces

- The largest monolithic active area of any pixel array
- No gaps due to the use of a single wafer-scale silicon sensor
- No charge sharing noise
- Zero counting losses
- High dynamic range
- High readout speed

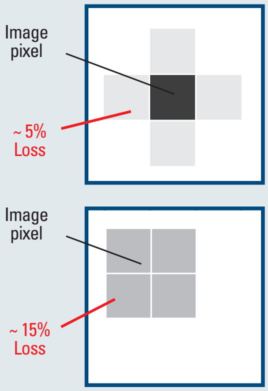
→ **Displayed image**



The pixel response from the detector to the displayed image is essentially perfect.

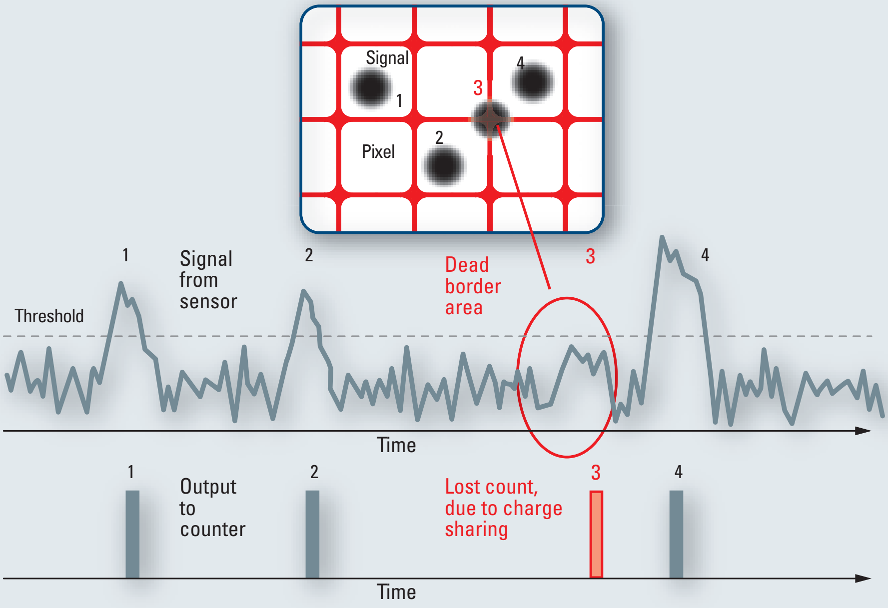
Blind Gap
Charge-Sharing
Threshold Loss

→ **Displayed image**



These “gaps” in the profile are not visible in the final image, since they are smaller than a pixel, but they cause the final intensity to be too low.

Charge sharing noise




IµS 3.0 X-ray source


METALJET X-ray source


PHOTON II CPAD

Microfocus Made Perfect: The IµS 3.0

Together with our partner Incoatec, Bruker pioneered the first modern microfocus sources. More than 750 of these outstanding sources have been installed in the field and have established an unequalled record for performance and reliability.

Now, with the new IµS 3.0, we take microfocus technology to the next level. It is the first ever microfocus source completely designed and optimized for crystallography.

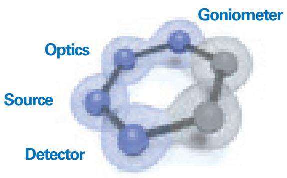
Other microfocus sources use technology that was designed for radiography or non-destructive testing (NDT). They are good when one needs to, for example, X-ray a pipe. However, for crystallography they fall short as much of the X-ray flux is simply wasted due to the non-optimal design.

Our IµS 3.0 is different; it is a completely new design fully tailored for crystallography. This means not a single compromise in performance, allowing the IµS 3.0 to achieve nearly twice the brilliance of other microfocus sources. Best of all, the IµS 3.0 features the same unique all-air-cooled operation and the same legendary reliability you have come to expect.

Beamline Intensities in your Home Lab, Exclusively from Bruker: METALJET

Bruker collaborated closely with Excillum during the development of the METALJET source, and with over five years of operational experience, Bruker has a deep understanding of the technology and offers by far the most advanced, experienced and reliable METALJET-based solutions. In the D8 VENTURE Second Generation, the METALJET is seamlessly integrated. By constantly monitoring all aspects of the source operation, our sophisticated firmware ensures ultra-stable long-term performance.

Finally, our unique, patented low-figure-error optics were specifically developed and optimized for the METALJET and are the only optics that fully preserve the inherent brilliance of the METALJET. Conversely, the relatively high-figure error of other multilayer optics typically leads to a loss of brilliance of up to 70%.



Our X-rays are "Green"

Top Performance & Light Footprint

With the D8 QUEST and D8 VENTURE, we are following design principles that protect the environment. Our PHOTON II detector and the advanced IµS 3.0 and METALJET sources all feature very low energy consumption and do not need water cooling. This significantly reduces carbon emissions and water consumption, improves reliability, and reduces the cost of ownership.

These benefits come with no compromises as all configurations feature unsurpassed performance.

saves
38 t of CO_2
per year *

No Water Supply

- Air-cooled PHOTON II
- Air-cooled IµS 3.0 microfocus source
- METALJET, no external cooling water required
- No external chillers required

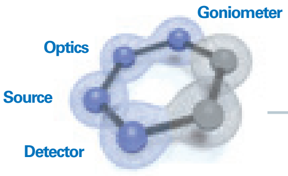
saves
5,200 m^3
cooling water
per year *

Single-Phase Power

- The PHOTON II has ultra-low power consumption
- The METALJET delivers beam intensities more than three times higher than microfocus rotating anodes, using only a fraction of a rotating anode's power consumption
- The IµS 3.0 uses 99% less energy than conventional rotating anodes
- Single-phase power and standard circuit breaker for ease of installation

saves
64,000 kWh
electrical energy
per year *

*) 24 hours, 300 days with IµS 3.0 and PHOTON II



D8 QUEST and D8 VENTURE: Systems as Individual as your Research

Sample alignment is easy and straightforward: large doors give you excellent access to the goniometer, and LED illumination guarantees perfect visibility of your crystal. Polarizing lenses and dimmable LED sample illumination greatly enhance crystal image quality. The crystal image is captured by a high-resolution video microscope that can be viewed remotely throughout the experiment.

Shutterless data collection with the D8 Structural Biology Solutions eliminates the need to repeatedly open and close the X-ray shutter… and the need to stop, reposition, and start the goniometer. During readout, conventional CCD and imaging-plate detectors require the mechanical shutter to be closed with the goniometer stopped, and then ramped back up to speed for the next exposure. As a result, mechanical jitter is introduced, adding significant systematic error to the data as well as wasteful overhead time to the experiment. In the D8 Structural Biology Solutions, the sample is constantly exposed to X-rays and continuously rotated, maximizing data acquisition efficiency and optimizing data quality.

The system's firmware provides the real-time status of the configuration and components that is not only used for efficient data collection planning, but is also carefully logged and safely stored with all other experiment information, ready to use for automated report generation and publications from your most sophisticated structure experiments.

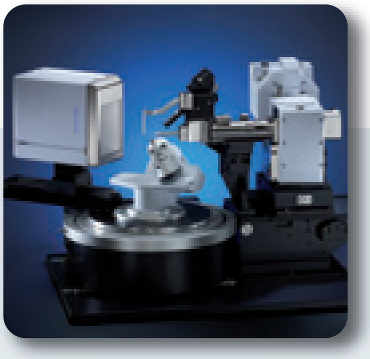
D8 QUEST and D8 VENTURE—a pioneering concept of flexibility and modularity.

D8 QUEST

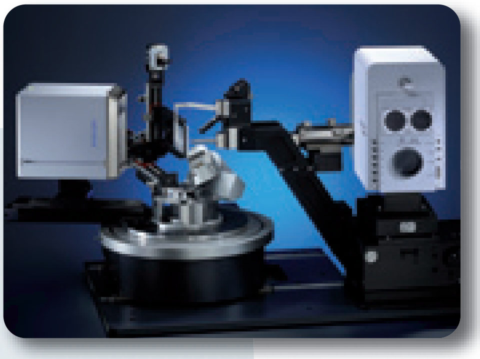
- Small footprint without compromises
- Accommodates IµS 3.0 configurations
- Exterior dimensions: 187 cm × 130 cm × 114 cm (h × w × d)

D8 VENTURE

- More room for more experimental flexibility
- Accommodates IμS 3.0, TXS, and METALJET configurations
- Exterior dimensions: 202 cm × 168 cm × 129 cm (h × w × d)



D8 VENTURE
configuration with:
- TXS source
- HELIOS MX optics
- KAPPA goniometer
- PHOTON II detector



D8 VENTURE
configuration with:
- METALJET source
- HELIOS MX optics
- KAPPA goniometer
- ISX stage
- PHOTON II detector

D8 QUEST compact
configuration with:
- IμS 3.0 source
- HELIOS MX optics
- KAPPA goniometer
- PHOTON II detector

D8 VENTURE
configuration with:
- METALJET source
- HELIOS MX optics
- KAPPA goniometer
- PHOTON II detector

Love KAPPA Geometry? We Invented it!

Bruker's four-axis KAPPA goniometer features an ergonomic, open-geometry design, offering:

- Easy sample mounting, harvesting, and monitoring
- Automatic detector-to-sample distance based on unit cell dimensions and crystal quality
- Large-unit-cell samples with the shortest detector-to-sample distance
- Friedel pairs on the same frame
- Optimum performance for in-house S-SAD phasing experiments
- Ultimate sample positioning freedom, for unconstrained multiplicity of observations
- Extremely high angular precision and fast goniometer positioning for productivity

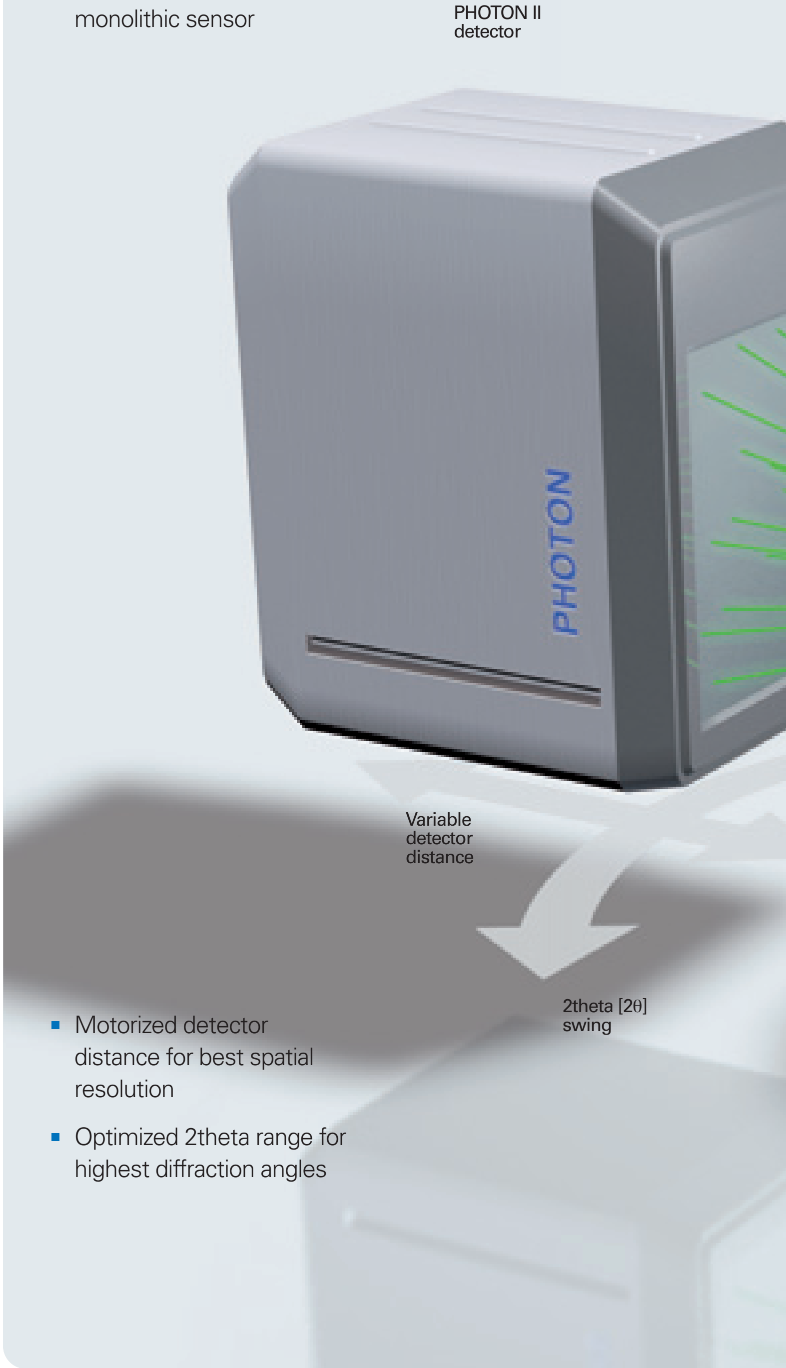
The same inspiration behind the KAPPA goniometer has also produced a new beam path. Designed for the easiest downstream alignment, and maximizing the accessible 2theta range for high-resolution work, the new beam path allows data resolution to the angstrom—or even better. The beam path design is mirrored by our new real-time path planning software, which combines 3-D models of the current hardware configuration with advanced trajectory algorithms for unprecedented goniometer control. Extensions with custom 3-D models are also possible, which makes it easy to add individual hardware.

The D8 QUEST and D8 VENTURE are both built for excellent sample access and visibility, and Bruker's KAPPA goniometer allows for easy sample mounting and retrieval. The absolutely open design protects your investment with maximum flexibility for future extensions.

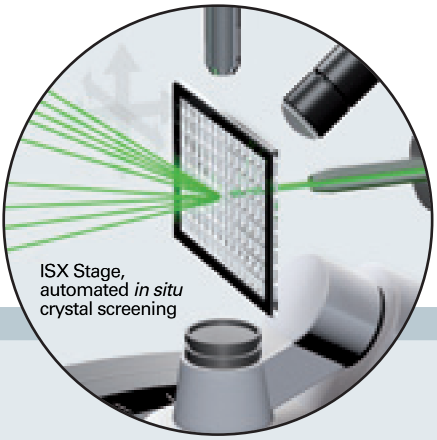
D8 Structural Biology Solutions—an abundance of unparalleled innovations.

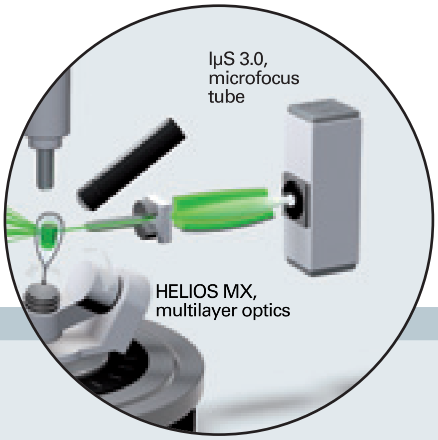
Diffractometer geometry

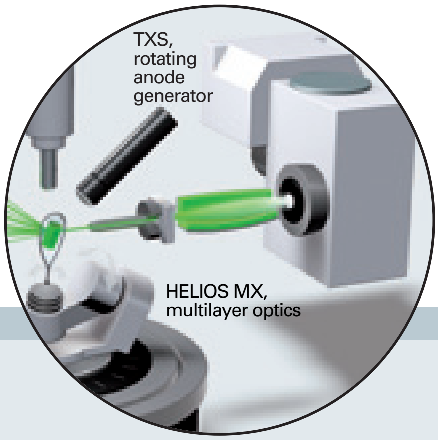
- PHOTON II detector with CPAD technology
- Large 140 cm^2 active area, monolithic sensor

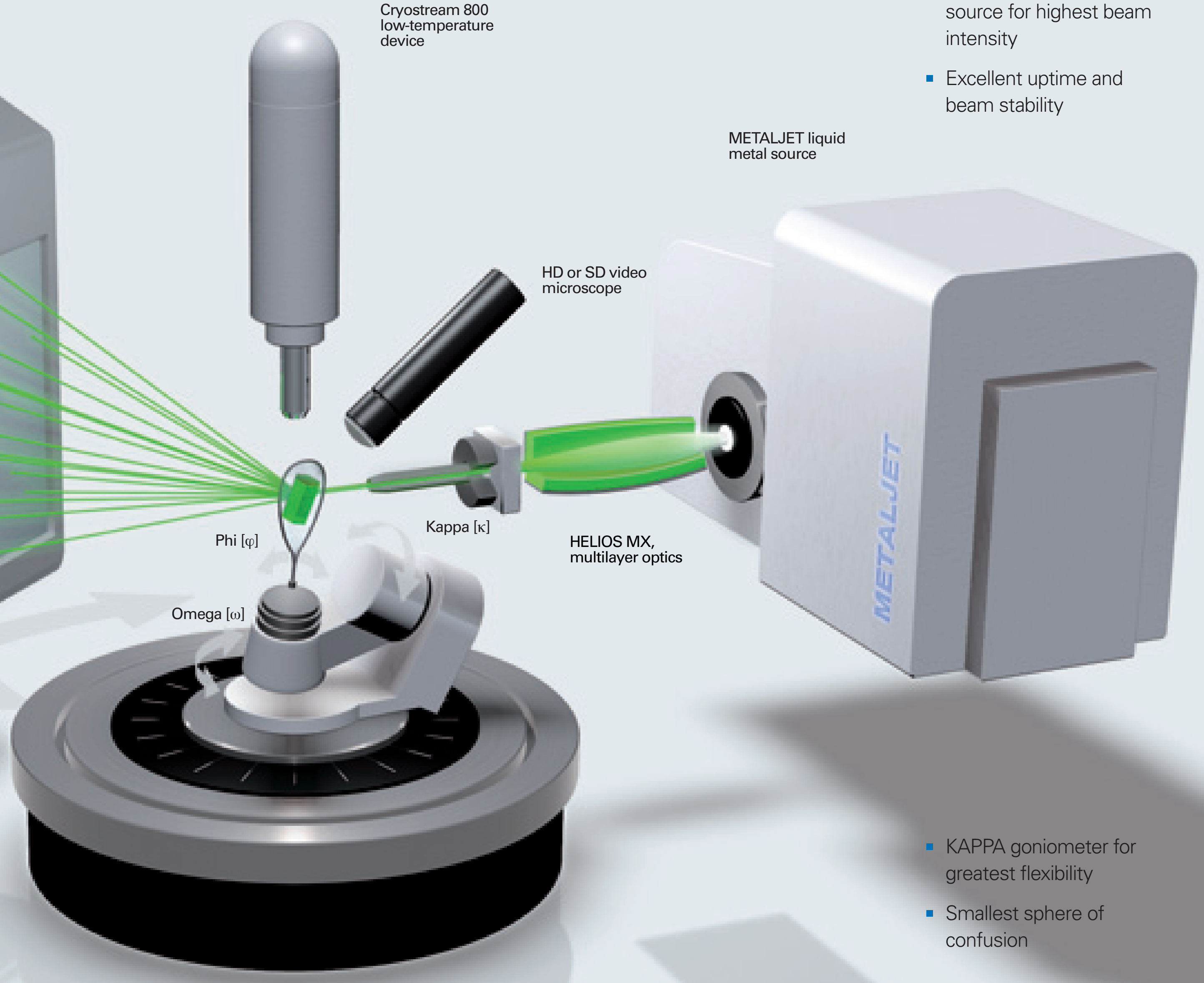


- Motorized detector distance for best spatial resolution
- Optimized 2theta range for highest diffraction angles









- METALJET liquid metal source for highest beam intensity
- Excellent uptime and beam stability

- KAPPA goniometer for greatest flexibility
- Smallest sphere of confusion

Good Diffraction Practice

The D8 Structural Biology Solutions are designed to the most stringent safety standards.

Conforms to:

- 2006/42/EC; 2006/95/EC; 2004/108/EC
- 96/29/EURATOM; RöV
- DIN EN 954-1 Cat. 3; DIN EN 61010-1/-2
- CSA C22.2 No. 1010
- EN 61000-6-1/-2/-3/-4

... and more

Approved by:

- TÜV
- NEMKO

IµS 3.0 with HELIOS MX

The IµS 3.0 microfocus source excels with low maintenance and high reliability.

- Twice the intensity of competitors' sources due to the first tube design tailored to the needs of crystallography
- Third-generation optics with superb accuracy, excellent reflectivity and precision
- Best spectral purity and a close-to-zero X-ray background
- Three-year source intensity warranty

TXS with HELIOS MX

Combined with the HELIOS MX optics, the compact TXS provides superb X-ray flux for in-house experiments on small protein crystals.

- Microfocus design with efficient resource management
- Excellent uptime and low maintenance costs due to long component lifetimes

ISX Stage

- Versatile stage for *in situ* plate screening that mounts on the KAPPA sample stage
- Fully-motorized plate stage for screening and data collection form multi-well plates
- Compatible with all SBS-format multi-well plates
- Access to all wells in one setting

Revolutionary Path Planning

- Revolutionary control software using advanced algorithms for optimized goniometer performance
- Software uses a 3-D model of the current hardware configuration for real-time path planning
- Extension with custom 3-D models is possible
- Component recognition

KAPPA Goniometer

The KAPPA 4-circle goniometer's open geometry offers ultimate sample positioning freedom, for unconstrained multiplicity of observations. The detector-to-sample distance is automatically optimized based on unit cell dimensions and crystal quality.

- Easy sample mounting and harvesting
- SNAP-LOCK mount for simple exchange
- Set of optimized collimators included

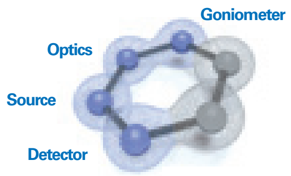
METALJET with HELIOS MX

The METALJET uses a liquid target consisting of a gallium-rich alloy.

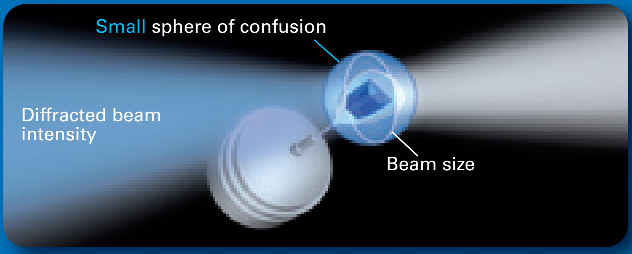
- Shorter-wavelength Ga-Kα radiation causes less radiation damage and facilitates high-multiplicity data sets
- The optimized HELIOS MX optics provides a beam optimized for the best signal-to-noise ratio
- Always fresh, self-healing target for high power load with long-term constant beam intensity

PHOTON II
Charge-Integrating Pixel Array Detector

- Largest monolithic active area: $140\ \text{cm}^2$
- Quantum-limited sensitivity
- High speed: up to 70 frames per second
- Zero readout dead time
- No nonlinearity at high count rates
- No charge sharing means better intensity



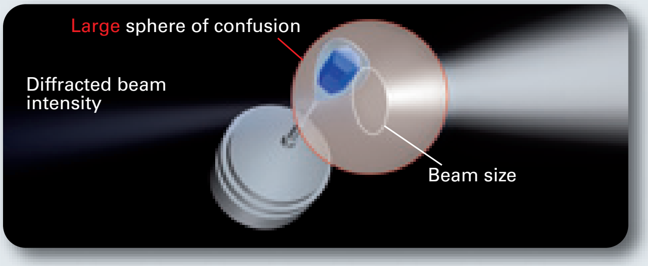
KAPPA Goniometer



Our D8 goniometer is designed for the highest accuracy and precision, superb alignment, and long-term reliability. The KAPPA has the smallest error in intersection of the instrument axes, providing the best sphere of confusion (SOC)—unsurpassed by any other goniometer. Even the smallest protein crystal stays reliably centered during the entire data acquisition, guaranteeing the best possible data.

- Sphere of confusion (SOC) < 7 micrometers
- Constant sample scattering volume in the beam
- Highest intensity from microcrystals

Conventional Goniometer



A large SOC is a serious problem since small crystals may completely move out of the beam. The smaller the beam and the smaller the crystal, the more pronounced this problem becomes. This significantly hampers correct scaling and results in systematically-poor data preventing, for example, successful S-SAD phasing experiments.

Patents and trademarks

Multiply-sampled CMOS sensor for X-ray diffraction measurements with corrections for non-ideal sensor behavior: Patent US 8,680,473

A method for correcting timing skew in X-ray data read out of an X-ray detector in a rolling shutter mode: Patent US 8,903,043

Method and apparatus for generating small size, high-intensity X-ray beams: Patent US 7,809,108

Method and device for aligning an optical element: Patent US 7,511,902

X-ray analysis instrument with adjustable aperture window: Patent US 7,983,388

X-ray optical configuration with two focusing elements: Patent US 8,345,822

Diffraction system for biological crystal screening: Patent US 6,836,532

Door configuration with a pivoting door and sliding door function which can be actuated by a single actuating element: Patent US 7,891,872 B2

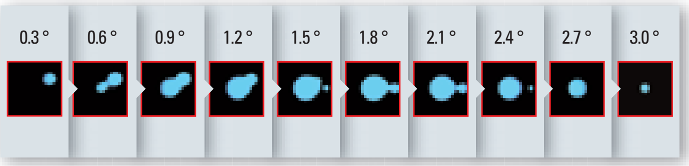
Patented low-figure-error optics specifically developed and optimized for the METALJET: Patent US 6,226,349

IµS is a trademark of Incoatec, Germany

Best Software = Best Structure = PROTEUM3

Slices every 0.3°

Fine slicing



Good profile

Our PROTEUM3 software guides you through the entire experiment with minimum input and maximum graphical feedback, and provides the most complete semi-automated pipeline: suggesting proper defaults whenever possible and asking for your expert decision whenever necessary. From quality assessment to phasing, PROTEUM3 is easy to use and lets you launch the underlying modules with a single mouse click. Stay informed about the progress and quality of the experiment via the intuitive GUI.

Use the world's best engines—all included in the suite—for crystal screening, data acquisition, data integration, and scaling to generate the best data for phasing.

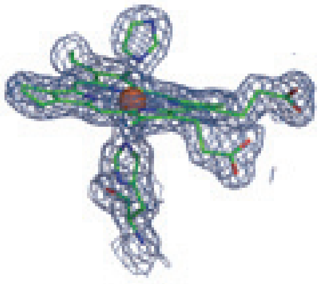
Benefit from built-in expert knowledge about instrument geometry and data collection strategies.

SAINT: From diffraction spots to accurate intensities.

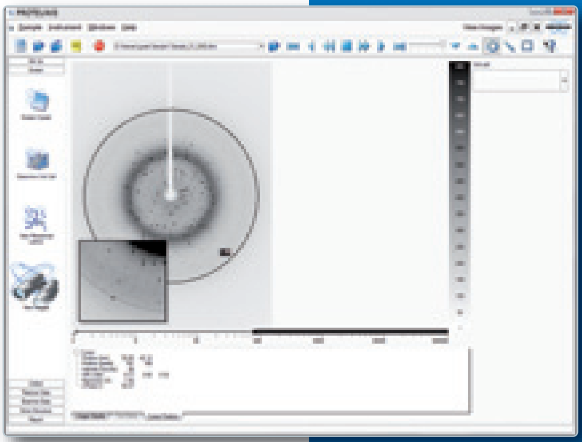
Reflections have a three-dimensional intensity distribution. Fine slicing is now the norm at synchrotron beamlines in order to preserve this information and thus improve signal-to-noise and data quality. Our software allows you to bring this powerful technique into the home lab by acquiring diffraction images in fine slices—a few tenths of a degree apiece. SAINT, our integration software, extracts the 3-D spot profiles and their intensity distribution, and learns 2theta-dependent profiles from strong, well-defined reflections in your data set. The software fits these learned profiles to weak reflections using least-squares methods, providing the best possible intensities. This approach makes a big difference—particularly for challenging samples—and our data quality always prevails.

Fine Slicing:
When the Anomalous
Signal Counts

- 3-D spot profiles and intensities are accurately extracted
- 2theta-dependent profiles are automatically "learned" from strong reflections
- "Learned profiles" are fit to weak reflections using least-squares methods
- More detailed density maps, easier tracing, and better structures



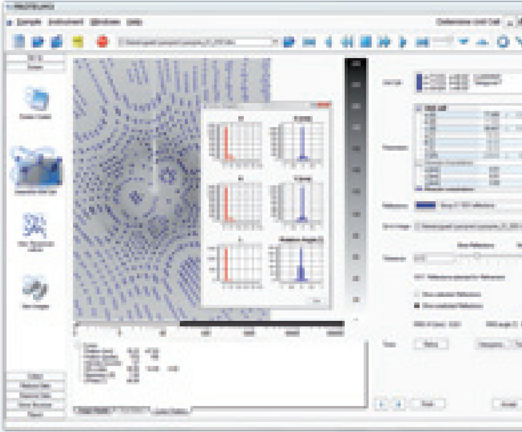
Metalloproteins
Kostan, J; Sjöblom, B; Maixner, F; Mlynek, G; Furtmüller, P G; Obinger, C; Wagner, M; Daims, H; Djinovic-Carugo K: J. Struct. Biol.
2010, **172**, 331

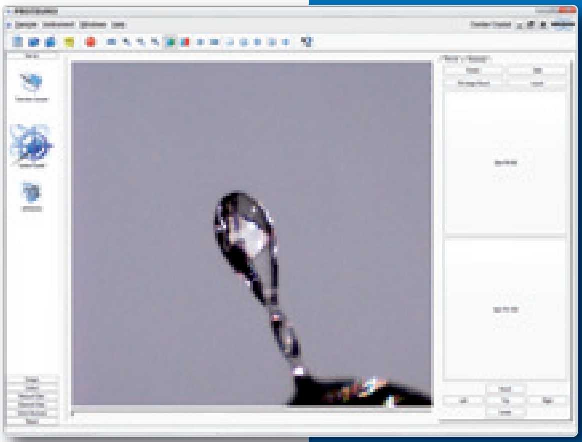


Crystal Screening

Preset or customer-defined crystal mounting positons combined with all required tools for frame analysis convert crystal screening from a tedious chore to a real pleasure.

Get fast and reliable feedback on the diffraction limits via resolution rings and spot separation.

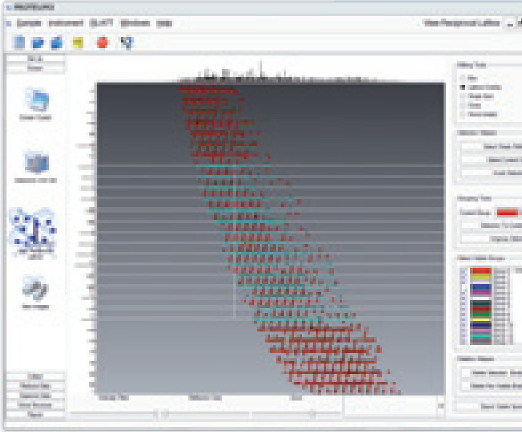




Crystal Snapshots and Movies

The excellent crystal illumination and high-resolution camera enable screen shots from the sample under investigation.

Pictures can be used for internal documentation, teaching or publication… or let the software take a movie.



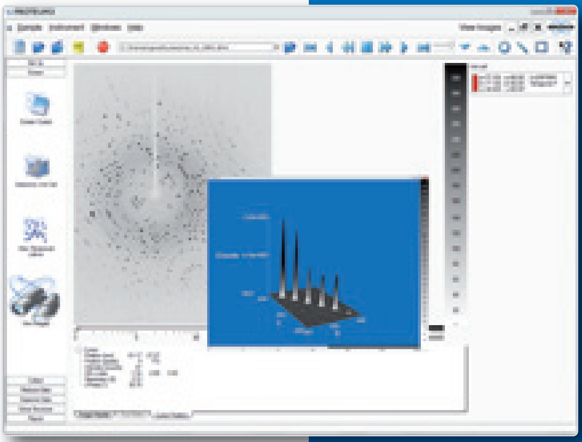
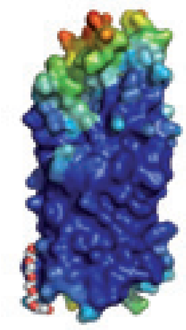


Image Analysis

The intuitive PROTEUM3 graphical interface provides all tools for image analysis including: zoom and panning, 3-D reflection profiles, line graphs, color schemes, movie mode, and many more…



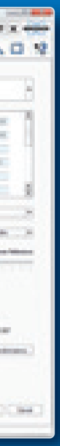
Membrane proteins

Prince, S M; Achtman, M;
Jeremy P. Derrick, J P:
PNAS
2002, **99**, 3417 *)

*) Plot created using data from the Protein Data Bank: Berman, H M; Westbrook, J; Feng, Z; Gilliland, G; Bhat, T N; Weissig, H; Shindyalov, I N; Bourne P E: Nucleic Acids Res. 2000, **28**, 235

Protein-DNA complexes

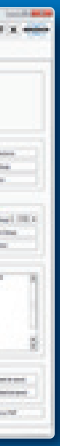
Fedorov, R; Witte, G; Urbanke, C;
Manstein, D J; Ute Curth, U:
Nucleic Acids Res.
2006, **34**, 670



Unit Cell Determination

An ingenious combination of fast Fourier and difference vector techniques indexes the most difficult data with absolute reliability.

Full nonlinear least-squares cell refinement with graphical feedback, overlay of spots, Bravais lattice determination, and tools for easy matrix manipulation complete this module.



Reciprocal Lattice Viewer

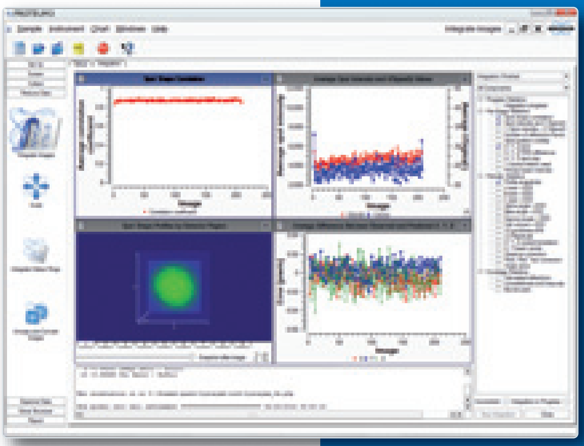
Display and interactively modify a reflection array for visual indexing. Remove artifacts for successful indexing.

A powerful tool for tackling twins and a great teaching tool.

Data Collection Strategy Planning

Specify multiplicity and the time you want your experiment finished, and the strategy planner will set up all required data scans for you!

The module provides statistical and graphical feedback.

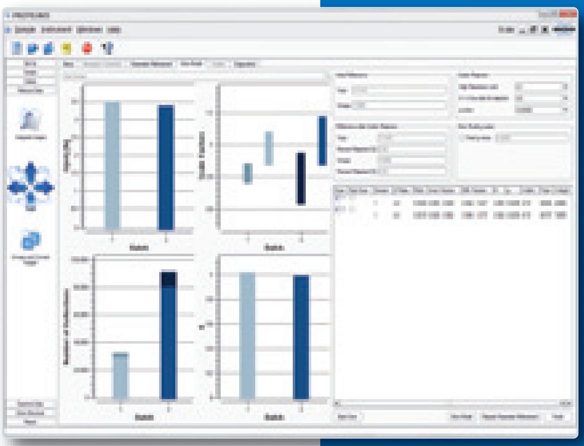


Data Integration

True 3-D integration with algorithms optimized for narrow scans.

The best software with on-the-fly integration and extensive feedback.

Includes the display of integration progress and quality, 3-D reflection profiles, multiple-component spot overlays, and many more.

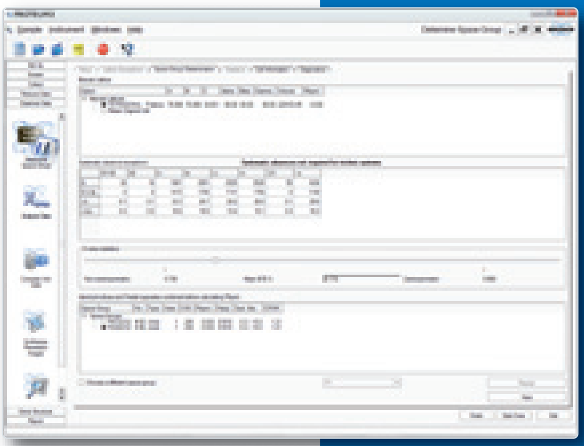


Data Scaling

SADABS and TWINABS are the perfect engines for scaling the data based on the intensities of symmetry-related reflections and data multiplicity.

The plugin handles single crystals and twins with graphical feedback and intelligent parameter suggestion, all transparent to the user.

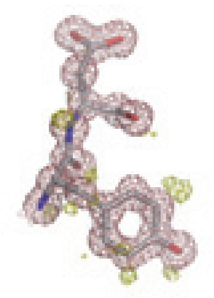
Fast and efficient.



Space Group Determination

Robust and reliable space group determination using a combination of lattice exceptions, systematic absences, and statistics to propose the correct space group.

Extensive data statistics and setup of files for structure solution are also provided.



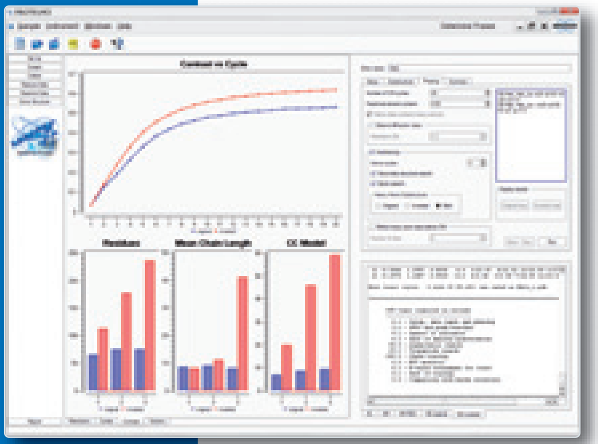
High-resolution structures

Benning, M:
2009, Lab Report SC-XRD 42,
DOC-L86-EXS042

Determine Phases

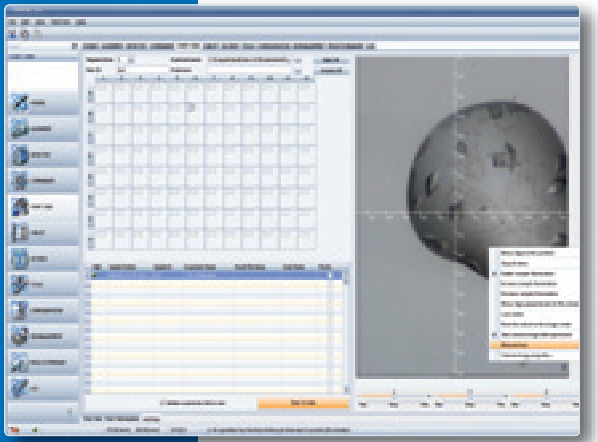
This module wraps around George Sheldrick's programs for solving the structure from SAD, SIR, SIRAS, MIRAS, and MAD data.

It provides easy parameter set up, graphical feedback, fast and reliable phasing, phase extension, and chain tracing.



ISX Stage

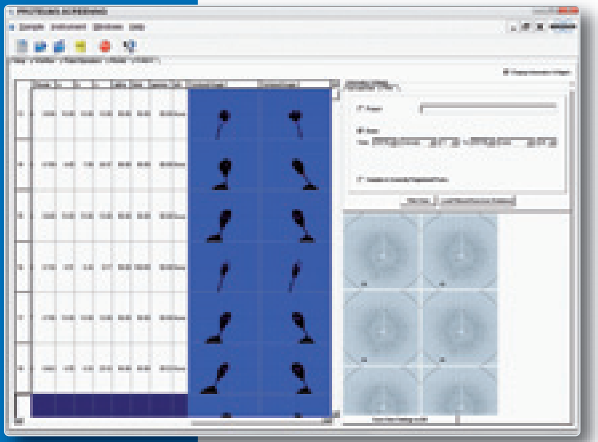
The ISX software is optimized for maximum productivity and ease of use. Job queuing allows for unattended screening of multiple samples.



PROTEUM3.SCREENING

An easy-to-use interface for screening experiments with automated scoring feedback drives the SCOUT robot.

The GUI makes it easy to select the best crystal for synchrotron data collection—or let the module collect the data for you.



PROTEUM3 Software Suite: Outstanding Tools for the Best Protein Structures

SADABS: The Champion for Fast Scaling.

SADABS is the fast and reliable solution for scaling of crystallographic data. During data collection with multi-axis instruments, the X-ray beam takes different pathways through the crystal, producing "true multiplicity". True multiplicity improves the quality of scaled data and allows a proper error analysis for accurate standard deviations of reflection intensities.

True multiplicity is of key importance for accurately extracting the anomalous signal for SAD phasing. TWINABS, the extension of SADABS, is the world's best solution for scaling protein data from twinned crystals.

XPREP: The Gold Standard for Space Group Determination.

Correct assignment of the space group is a prerequisite for structure solution and refinement. The highly-advanced space group determination engine XPREP has all required tools built in. It is easy to use and has all required tools built in, including merging data from various data sets, statistical analysis, display of calculated Patterson sections, de-twinning of merohedral crystals, and much more.

SHELXTL™: The Phase Problem Disappears.

SHELXTL™ is the extended, proprietary version of Professor George Sheldrick's SHELX. Two of its modules, XM and XE, form the core for solving the structure from anomalous data, such as SIR, SAD, SIRAS, MIRAS, or MAD.

While the XM module does a perfect job providing the initial phases, the XE engine accomplishes the phase extension and uses the low-density elimination approach to resolve the twofold ambiguity. XE is renowned as extremely fast, robust, and easy to use—features that facilitate its use in high-throughput structure centers. The very efficient chain-tracing feature makes XE a perfect engine for your structural research.

Report Generation Made Easy.

PROTEUM3's flexible, template-based report generation function has automated the tedious task of writing reports. The HTML report summarizes all experimental information along with results from data integration, scaling, space group determination, and chain tracing.

PROTEUM3: Open to the Outside World.

PROTEUM3 offers export options to other programs at various points in the workflow, facilitating the use of other crystallographic programs and maintaining your laboratory's established data processing sequence. Conversely, PROTEUM3 provides import options for various data and diffraction image formats for the use of PROTEUM3 with external data. In particular, PROTEUM3 features native support of CBF and XDS formats.

PROTEUM3: Easy to use for the Novice, with all the Features for the Experts!

Automation Tools: Exploit the Full Power of your D8 System

SCOUT sample changer

ISX screening stage

The extreme brightness of our D8 Structural Biology Solutions makes high throughput screening now more practical than ever. Bruker offers advanced automation tools to efficiently screen crystallization plates or frozen samples from pucks in dewars.

SCOUT sample changer: High Throughput meets High Reliability.

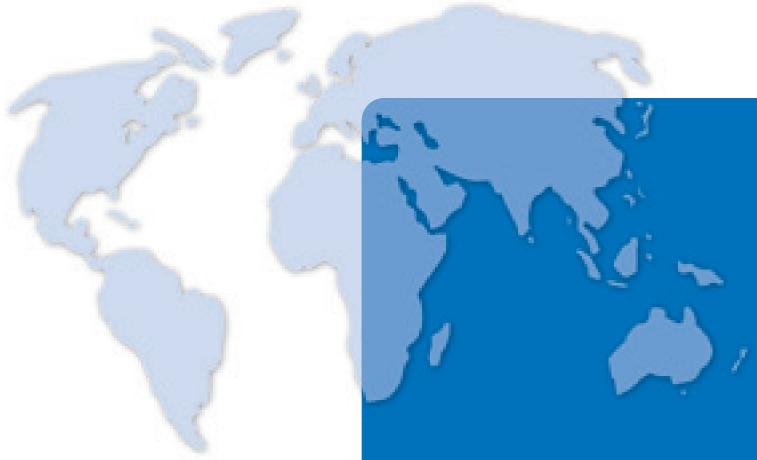
The SCOUT sample changing robot combines proven hardware with a powerful user interface developed in collaboration with the Structural Genomics Centre at Oxford University.

The most important feature of SCOUT is outstanding reliability. SCOUT is also the only sample changing robot that meets all the latest CE safety certification requirements.

ISX Stage: *In situ* Plate Screening Made Easy.

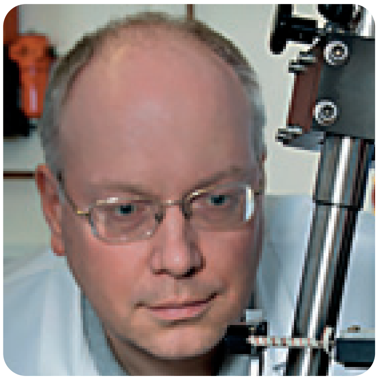
Many more researchers are now interested in screening crystal diffraction quality within the crystallization plate. The ISX stage is a powerful new tool, both for screening crystals and for collecting room-temperature data using the latest serial crystallography techniques—recently pioneered at synchrotron beamlines.

The ISX is completely motorized. It mounts easily onto the KAPPA goniometer using a kinematic mount, so it can be installed within minutes and then simply removed after use to continue standard operation with frozen samples.



Dr. Dima Chirgadze
Head of The Crystallographic X-ray Facility at the Department of Biochemistry, University of Cambridge; United Kingdom

"The quality of the data coming off the machine is very high, easily beating anything we had collected ever before on an in-house X-ray source. This gave us the possibility to accurately measure the very small Sulphur anomalous signal for our SAD experiments. We now routinely use structure solution by SAD and have obtained ab-initio phases for over a dozen crystal structures, including a new form of DNA by P-SAD."



Dr. Jérôme Basquin
Crystallization Facility, Max-Planck-Institute for Biochemistry (MPI Biochem), Martinsried, Germany

"Despite having regular access to synchrotron beam lines, we felt it was important to have a powerful in-house system. This new system was initially intended to screen small or poorly diffracting crystals and guide us to select and rank our samples to maximize our efficiency at the synchrotron. Fortunately, we got the chance to thoroughly test the D8 VENTURE system on our challenging targets. From the results seen we were convinced that the METALJET high intensity source would fulfil our requirements. Despite our initial reservations about opting for a novel technology, we decided to become the first installation of the D8 VENTURE with METALJET single crystal diffraction system in Europe.

Today, six months after the system installation, the performance of the METALJET system impresses us daily and the system is exceeding our expectations."

Welcome to the Bruker User Group

Using a Bruker system gives you instant access to the Bruker SC-XRD User Group, a global scientific network linking scientists from more than 1,300 Bruker installations. With the introduction of 2-D electronic detectors for the home lab, our customers started this group which has grown to more than 600 members, including a large number of world-class crystallographers.

The group is actively exchanging hints and tips. As these are global groups, you can expect replies virtually 24/7, with someone always reading the mails somewhere. In practice, this means that urgent questions can be answered almost instantly and your research can progress without delay. Become part of the global Bruker family in crystallography, and join the community of Bruker users.

Overview of Features and Benefits

Detector	Feature	Specification	Benefit
PHOTON II	Fourth generation Charge Integrating Pixel Array	Latest pixel array detector technology	Higher speed and sensitivity, best data quality
	Large active area	100 × 140 mm^2	Faster data collection
	High readout frequency	70 Hz	
	Readout dead time	0 sec (full shutterless operation)	
	High sensitivity	Single photon detection	Improved data quality
	No dead areas	Single, monolithic silicon sensor	
	No charge sharing noise	0 electrons charge sharing noise	
	No parallax	< 0.1 pixel (for Cu, Ga)	
	No count-rate nonlinearity	< 1% nonlinearity up to full count rate	
	High detective quantum efficiency (DQE)	> 90% Cu	
	No operating gas or cooling water	Completely sealed, air-cooled design	No maintenance, high uptime
	High reliability	Warrantied for 3 years	
Sources	Feature	Wavelength	Benefit
IμS 3.0	Twice the brightness of competing microfocus sources	Guaranteed intensity: 2.4 [10^{10} photons / s · mm^2], Cu-Kα, 1.54 Å	Best-in-class performance
	No routine maintenance, high reliability	3-year warranty	Costs of ownership close to zero
TXS	Very high-intensity beam, rotating anode	Guaranteed intensity: 16.0 [10^{10} photons / s · mm^2], Cu-Kα, 1.54 Å	Higher performance for small, weakly diffracting samples
	Pre-aligned and pre-crystallized filament cassettes		Unprecedented ease-of-use, longest uptimes, and maximum productivity
METALJET	Highest intensity beam powered by liquid-metal jet technology	Guaranteed intensity: 35.0 [10^{10} photons / s · mm^2], Ga-Kα, 1.34 Å	Ultimate performance for small, poor-crystallinity samples
	Metal jet continuously supplies fresh target material		Long-term beam stability
Goniometer	Feature	Specification	Benefit
KAPPA	Very low sphere of confusion	< 7 μm	Best data quality
	Kappa geometry	Highest flexibility	
	High speed	Up to 1,200 deg/min (omega)	Faster data collection
Automation	Feature	Specification	Benefit
SCOUT sample changer	Reliable, small-footprint cryo-cooled protein crystal handling unit for automated crystal screening and data collection	Six-axis robot with auto-refill sample dewar	Enhances system's throughput, ideal for identifying best crystals before a synchrotron trip
ISX screening stage	Versatile stage for *in situ* plate screening	Compatible with all SBS-format multi-well plates, with access to all wells in one setting	Identifies your best crystals, and collects complete data sets at room temperature

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