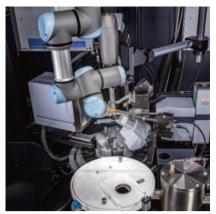


### MACROMOLECULAR CRYSTALLOGRAPHY D8 VENTURE D8 QUEST

High-end Solutions for X-ray Crystallography Innovation with Integrity



IµS DIAMOND II: Rotating anode performance



SCOUT: Automated cryo-cooled protein crystal handling



Low temperature attachment





Stable and easy-to-align beam path



METALJET D2 PLUS: the most intense home source



Wide doors for easy access



PHOTON III photon-counting detector with large active area





Metalloproteins 1)

## X-ray Crystallography drives Structural Biology forward

The field of structural biology continues to advance dramatically with researchers tackling ever more complex and challenging macromolecular structures. X-ray crystallography, the engine of this ongoing quest, is accounting for over 75% of the structures deposited in the Protein Data Bank since 2020.

The best in-house X-ray systems provide the fastest and most economical route to protein structures for increasingly challenging problems, such as large protein complexes and tiny crystals.

#### Great research deserves great tools.

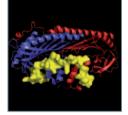
As structural biology advances, the need for fast, economical structure determination is becoming more acute. Modern laboratories, whether in academic research or commercial drug-discovery, need better crystallographic instruments in-house – more powerful, faster and much easier to use.

At Bruker, our driving passion is to provide scientists with highest-quality tools for crystallography. With this goal in mind, our research and development teams are continuously pushing the frontiers of innovation, helping you get better structures faster with greatly increased efficiency. These efforts resulted in a range of highly advanced home-lab instruments:

Third-generation Macromolecular Crystallography Solutions – D8 QUEST and D8 VENTURE.



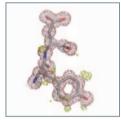
Molecular motors <sup>4)</sup>



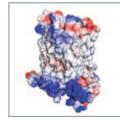
High-throughput crystallography <sup>7)</sup>



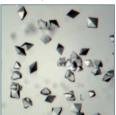
High-resolution structures <sup>10)</sup>



GPCR crystallography <sup>13)</sup>



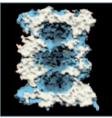
#### Microcrystals<sup>2)</sup>



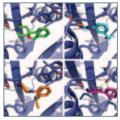
Structural proteins and scaffolds 5)



Protein complexes <sup>8)</sup>



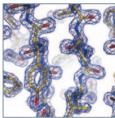
Fragment-based lead generation 11)



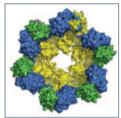
Protein-protein interactions 14)



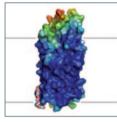
SAD phasing 3)



Multi-protein complexes 6)



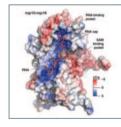
Membrane proteins 9)



Molecular replacement 12)



Viral protein-RNA structures <sup>15)</sup>



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### Brighten up your home lab with IµS DIAMOND II or METALJET D2 PLUS

IµS DIAMOND II X-ray source with HELIOS optics

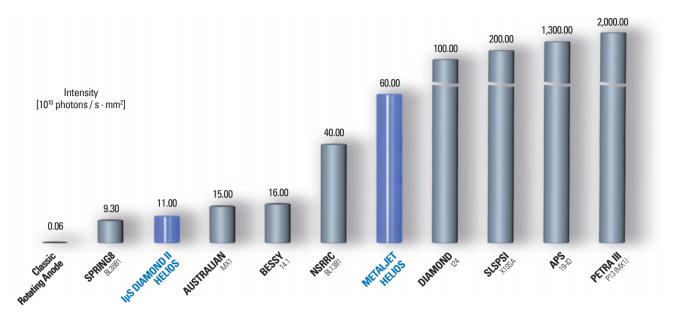
High flux, stability, small beam size, and low divergence are essential for collecting high-quality data from challenging crystals. These requirements have driven developments in synchrotron design. Now, Bruker has applied these important principles to home-lab source technology. Our sources deliver beam intensities comparable to those of typical bending-magnet beamlines. The modern METALJET D2 PLUS 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.

#### 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 I $\mu$ S DIAMOND II, 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.

Gallium: the better copper.

### Home Sources vs. Bending Magnet Beamlines



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

### IµS DIAMOND II: sealed tube convenience, rotating anode performance.

With over 1,700 systems installed in the 20 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.

All our  $\mu$ S sources are developed completely and specifically for crystallography which results in higher intensity than any other microfocus source. However, there is more we can do: diamond hybrid anode technology, with an eight times better heat conductivity than copper, allows a further increase in the power load, leading to the  $\mu$ S DIAMOND, a source outperforming modern microfocus rotating anodes.

The second generation, the I $\mu$ S DIAMOND II, pushes the limits in microfocus source technology for biological crystallography even further. The I $\mu$ S DIAMOND II features isotopically pure diamond, which has the highest thermal conductivity of any known material. A new high-brightness cathode produces a more homogenous, higher current density electron beam. Both improvements allow a power load increased once more, leading to ultimate X-ray intensities and making conventional microfocus rotating anode generators obsolete. Even better, the I $\mu$ S DIAMOND II has essentially no maintenance costs or downtime. We support every single unit with a three-year warranty.

IµS DIAMOND II - simply brilliant.

### METALJET D2 PLUS with our best HELIOS optics

#### The X-ray revolution without rotation.

The METALJET D2 PLUS 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 DIAMOND II, the METALJET D2 PLUS is operated with single-phase power and also requires no external cooling, minimizing installation requirements.

### HELIOS MX: the brightest optics under the sun.

Our HELIOS multilayer optic delivers up to three times the intensity of conventional multilayer optics. Improved deposition technology yields higher precision and greatly enhances the optic's reflectivity.

For the METALJET D2 PLUS, 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 source. Conversely, a METALJET combined with a conventional, relatively highfigure-error multilayer optic typically leads to a loss of brilliance of up to 70%.

#### **Collimators for beam optimzation.**

The highly-monochromatic X-ray beam provided by the HELIOS optics can be easily and reproducibl optimized to match the characteristics of each sample. A set of collimators control beam size and divergence and is an integral part of each D8 QUEST and D8 VENTURE system.



Liquid metal METALJET D2 PLUS with HELIOS optics

### Our X-rays are "Green"



#### **Future-Proof Solutions**

With the D8 QUEST and D8 VENTURE, we are following design principles that protect the environment. Our PHOTON III detector and advanced IµS DIAMOND II and METALJET D2 PLUS 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.

#### Saves 26 t of CO<sub>2</sub> per year \*



#### **No Water Supply**

- Air-cooled PHOTON III
- Air-cooled IµS DIAMOND II microfocus source
- METALJET D2 PLUS, no external cooling water required

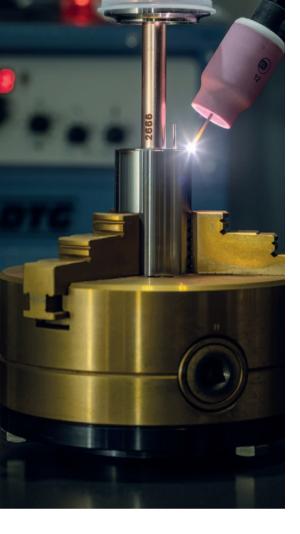
Saves 1,700 m<sup>3</sup> cooling water per year \*



#### **Single-Phase Power**

- Ultra-low power consumption of all PHOTON III detectors
- IµS DIAMOND II uses
   99% less energy than conventional rotating anodes
- METALJET D2 PLUS delivers beam intensities more than three times higher than microfocus rotating anodes, using only a fraction of a rotating anode's power consumption
- Single-phase power and standard circuit breaker for ease of installation

Saves 43,000 kWh electrical energy per year \*

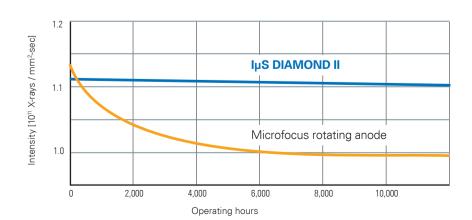


### An entire tube production line – for the best IµS sources

All IµS tubes are designed, developed and manufactured exclusively by Incoatec. Indeed, Incoatec is the only company that makes microfocus tubes optimized for X-ray diffraction. These optimized tubes offer higher performance and higher quality, resulting in longer tube lifetimes.

Source	Typical tube lifetime	Relative intensity
Bruker IµS DIAMOND II	5 years	1.1
Microfocus rotating anode	1 year	1.0 *)

\*) with fresh anode only



In contrast to rotating anodes, the heat load on the IµS DIAMOND II surface is constant over time, making the output of the IµS DIAMOND II much more stable. The IµS DIAMOND II source also outperforms microfocus rotating anodes without the headache of high running costs and without routine maintenance.



#### IµS DIAMOND II for Cu radiation

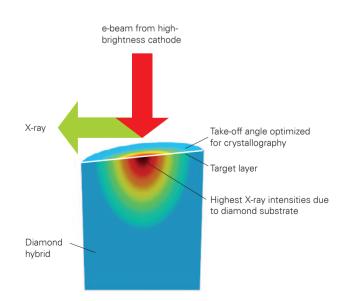
- The average intensity is 20% higher than that of a microfocus rotating anode source. The best optics put all the X-rays on the sample for up to 10 times lower scattered X-ray background.
- Unique 99% uptime guarantee.
- 10 times better stability than rotating anodes for the best data quality.



### METALJET D2 PLUS with HELIOS for Ga radiation

- The METALJET D2 PLUS uses a liquid target consisting of a Gallium rich alloy.
- Compared to Cu radiation, Ga-Kα radiation allows higher multiplicity data sets in less time.
- Fresh, self-healing target for high power load with long-term constant beam intensity.

### IµS DIAMOND II hybrid anode



Higher intensities are achieved in the I $\mu$ S DIAMOND II by optimizing all the critical tube parts, such as the cathode, electron optics and take-off angles.

In addition, the diamond hybrid anode used in the IµS DIAMOND II features an isotopically pure diamond substrate that is coated with a layer of the target material and thus takes advantage of the high thermal conductivity of diamond to achieve even higher intensities.

The high-brightness cathode provides the most homogeneous electron-beam with the highest intensity of any microfocus tube.



The PHOTON III is available in three different sizes, perfectly matching the requirements of your application.

PHOTON III: Large active-area, photon-counting detector – no photon is left behind



The best crystal structures for publication require large active-area X-ray detectors with high signal-to-noise ratios for accurate weak and strong reflection intensities.

### Our PHOTON III family matches these requirements perfectly:

- The largest active area available in an in-house detector with no gaps or dead areas.
- True photon-counting detection for the accurate measurement of weak reflections.
- Operation in charge-integration mode eliminates pulse pileup and charge sharing noise.

#### The latest generation of detectors for synchrotrons and XFELs uses a new, improved technique for photon counting based on charge integration.

These new charge-integrating detectors, such as the JUNGFRAU (SWISSFEL) and the ePIX (LCLS), do not suffer anymore from pulse pileup or charge-sharing noise and thus have proven to produce markedly superior data compared to conventional Hybrid Photon-Counting (HPC) detectors. The PHOTON III is the first in-house detector based on this latest charge-integration technology. The PHOTON III thus features zero detector noise and also eliminates charge sharing and pulse pileup noise that plague conventional HPCs.

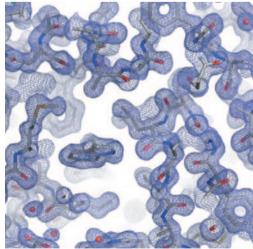
The PHOTON III also features an advanced rare-earth X-ray convertor that has up to three times the Detective Quantum Efficiency of silicon sensors.

The unique combination of these features makes the PHOTON III the best in-house detector.

Lysozyme electron density map from the PHOTON III dataset refined to 1.55 Å, contoured at 1s.

The PHOTON III employs large monolithic sensors and therefore has no dead areas or blind gaps: 100% of the surface is fully sensitive to X-rays.





# PHOTON III: Large active area – no gaps

- Largest active area for highest redundancy
- No gaps or dead areas
- Charge integration for best linearity
- Photon-counting for best sensitivity
- High dynamic range
- All air-cooled



#### Best Data

The PHOTON III is the only laboratory detector featuring the latest chargeintegrating, photon-counting technology. It excels at both weak and strong reflections, ensuring superior data.



#### **Highest Quality**

Three-year warranty, air-cooling and no maintenance go hand in hand to deliver a long-lasting, highly reliable detector.



#### No blind areas

PHOTON III detectors feature large monolithic sensors. Even multimodular versions do not suffer from dead areas between the sensors. This allows faster data collection and greater completeness.



#### **Outstanding linearity**

Charge integration means no pulse pileup noise and thus the best linearity for strong reflections.



The photon-counting PHOTON III detector delivers outstanding data quality from even the most challenging samples.



#### Large Active Area

The PHOTON III offers the largest active area for the home laboratory – letting you capture more reflections in just one detector setting and get better separation of closely spaced reflections.

Y	

#### **High Speed**

With a detector frame rate of 70 Hz, zero readout dead time and shutterless operation, data are acquired quickly and accurately.



#### **Charge Integration**

Charge integrating detectors record a very high speed 'movie' of the diffraction pattern. A fast processor then looks for X-ray 'hits' in each frame of the movie. The result: photon counting with no charge sharing or pulse pileup noise for optimal data quality.

### Love KAPPA geometry? Perfect, we invented it!

Low-temperature device

Карра [к]

Phi [φ]

Omega [ω]

Video microscope

HELIOS

multilayer optics

- PHOTON III detector photon-counting CPAD technology
- Large, up to 280 cm<sup>2</sup> active area, no gaps

PHOTON III detector

PHOTON

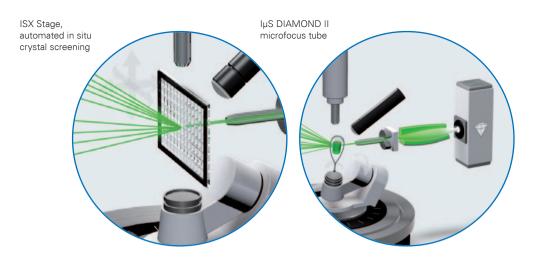
Variable detector distance

2theta [20] swing

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

- KAPPA goniometer for greatest flexibility

- Smallest sphere of confusion



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

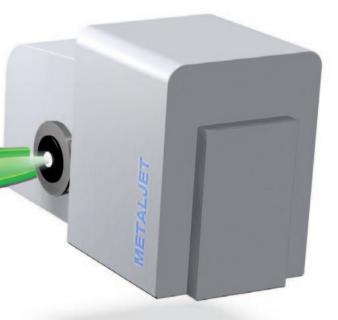
- Easy sample mounting, harvesting, and monitoring.
- Automatic detector-to-sample distance based on unit cell dimensions and crystal quality.
- Large-unit-cell samples with the shortest detector-to-sample distance.
- Friedel pairs on the same frame.
- Optimum performance for in-house S-SAD phasing experiments.
- 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.

METALJET D2 PLUS liquid metal source



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

#### **D8 QUEST**

- Small footprint
  - without compromises Accommodates
- IµS DIAMOND II configurations
- Exterior dimensions: 187 cm  $\times$  130 cm  $\times$  114 cm (h  $\times$  w  $\times$  d)

Configuration example:

- IµS DIAMOND II source
- HELIOS optics
- KAPPA goniometer
- PHOTON III detector

### D8 QUEST and D8 VENTURE: Systems as individual as your research

Sample mounting and alignment are 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 and can be viewed remotely throughout the experiment.

With our D8 Macromolecular Solutions, we offer a pioneering diffractometer concept with flexibility and modularity. The D8 QUEST and D8 VENTURE can be perfectly configured for the demands of any imaginable application in protein single crystal X-ray diffraction.

#### Just follow three simple steps:

- Choose your preferred X-ray source and optics and combine it with the best KAPPA goniometer.
- 2. Add the state-of-the-art photon-counting PHOTON III detector with an active area fitting your needs.
- 3. Complete your system with accessories, such as the ISX stage or the SCOUT sample changing robot.

Now you are ready to run the most sophisticated experiments.

While the experiment is in progress, your sample is constantly exposed to X-rays and continuously rotated, maximizing data acquisition efficiency and optimizing data quality. Finally, 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 VENTURE**

- More room for more experimental flexibility
- Accommodates IµS DIAMOND II or METALJET D2 PLUS configurations
- Exterior dimensions:
   202 cm × 168 cm × 129 cm (h × w × d)

#### Configuration example:

- METALJET D2 PLUS source
- HELIOS optics
- KAPPA goniometer
- PHOTON III detector







### Automation tools: Unleash the full power of your D8 System

#### Make your sample get to the point!

Small crystals and small X-ray beams require ultra-accurate centering, which pushes mechanical goniometer heads to their limits with respect to accuracy, precision, and backlash. Our automated goniometer head (AGH) is a masterpiece of electronics and mechanical engineering with its high level of miniaturization, precision, and reliability. It allows fully automatic centering of your magnetic-pin-mounted sample.

#### SCOUT sample changer: high throughput meets high reliability.

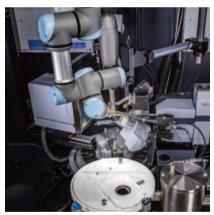
The SCOUT sample changing robot combines proven hardware with a powerful user interface. A robust piezo-driven automated goniometer head ensures accurate automated centering of the sample in the X-ray beam. The most important feature of SCOUT is its outstanding reliability. SCOUT meets all the latest CE safety certification requirements for automated operation.

#### ISX stage: in-situ plate screening made easy.

Many researchers are now interested in screening crystal diffraction guality 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 cryo-cooled samples.



AGH for fully automated sample centering



SCOUT: Automated cryo-cooled protein crystal handling



ISX Stage: Automated in-situ crystal screening



## Ultimate ease-of-use, highest flexibility – PROTEUM

Our PROTEUM 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, PROTEUM 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.

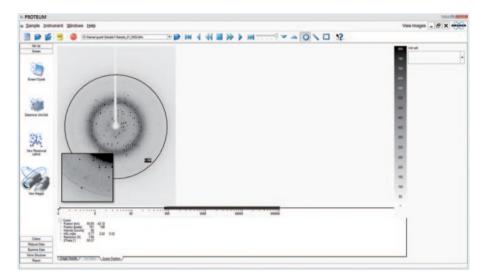
Benefit from built-in expert knowledge about instrument geometry and data collection strategies.



#### **Crystal Screening**

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

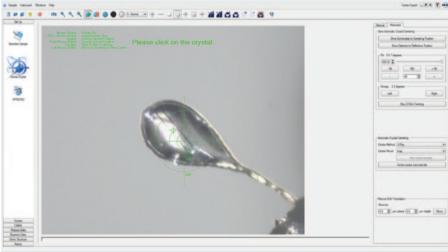
Get fast and reliable feedback on the diffraction limits via resolution rings and spot separation.



#### **Crystal Snapshots and Movies**

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

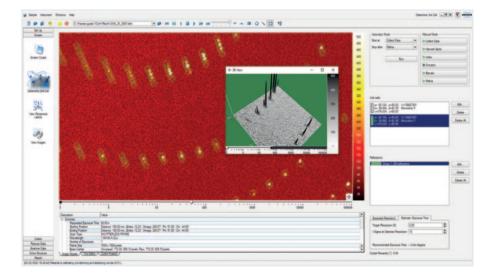
Pictures can be used for internal documentation, teaching or publication... or let the software take a movie.

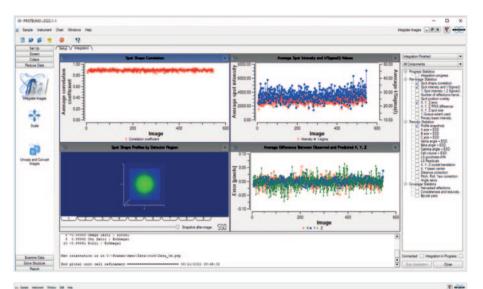


#### Unit Cell Determination

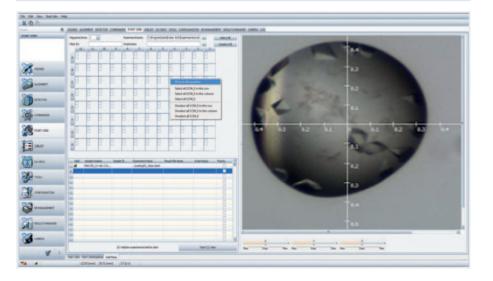
An ingenious combination of fast Fourier and difference vector techniques indexes the most difficult data with absolute reliability.

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









#### **Data Integration**

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

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

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

#### **PROTEUM.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 plug-in collect the data for you.

#### **ISX Stage**

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

aim 03011

#### **Overview of Features and Benefits**

	Feature		Benefit	
	Photon-counting pixel-array detector	5th generation pixel array detector technology	Higher speed and sensitivity, best data quality	
	Large active area	100 × 70 mm <sup>2</sup> 100 × 140 mm <sup>2</sup> 200 × 140 mm <sup>2</sup>	Higher data redundancy, minimized background scatter	
	Fast readout time	14 msec	Faster data collection	
	Very high countrate	Up to $4 \times 10^6$ counts/pixel-sec		
	Readout dead time	0 sec (full shutterless operation)	<ul> <li>Superior data precision</li> </ul>	
	Monolithic silicon sensors		No gaps, no dead areas	
PHOTON III Detector	High dynamic range		No reflection overloads	
	Mixed mode, integrating detection		More accurate reflection intensities	
	Small pixel size, minimized point-spread		Best long axis resolution, best spot separation	
	High count-rate linearity	< 1% nonlinearity up to full count rate	Better <i>R</i> -factors	
	High detective quantum efficiency (DQE)			
	No operating gas or cooling water	Completely sealed design, air-cooled	No maintenance, high uptime	
	High reliability	Warrantied for 3 years		
IµS DIAMOND II Source	Very high intensity beam, completely aircooled, revolutionary cooling technology	Cu radiation	Rotating performance from a microfocus sealed tube, ultra-low maintenance, optional dual-wavelength configuration	
METALJET D2 PLUS Source	Highest intensity beam	Ga radiation	Ultimate performance for small, weakly diffracting samples	
D8 Goniometer	Very low sphere of confusion	< 7 µm	Best data quality	
	Kappa geometry	Highest flexibility	Easy sample mounting	
	High speed	Up to 1,200 deg/min (omega)	Faster data collection	
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 crystal 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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