

# Structural Biology

Single crystal X-ray diffraction and SAXS

Systems designed for structural biology



**Rigaku**  
oxford diffraction

# Rigaku Oxford Diffraction

## THE POWER OF SYNERGY

Combining the single crystal groups from Rigaku and Oxford Diffraction has produced an organization that is uniquely positioned to provide the best combination of technologies for your structural biology needs.



## DETECTOR OPTIONS

Detector technology has often been a key driver in the advancement of X-ray crystallography research. Rigaku Oxford Diffraction's systems are offered with hybrid photon counting (HPC) detectors, such as Rigaku's HyPix-6000 and Dectris's PILATUS and EIGER detectors that are known for high dynamic range, fast readout and essentially no noise. HPC detectors provide outstanding performance for macromolecular crystallography experiments.

Source	Source type	Power loading	Dual wavelength capability?
MicroMax™-003	Microfocus sealed tube	30 W	No
MicroMax-007 HF	Microfocus rotating anode	1.2 kW	Yes
FR-X	Microfocus rotating anode	2.970 kW	Yes

## X-RAY SOURCES

Rigaku Oxford Diffraction offers several sources to fit the needs of your experimental samples and throughput including a microfocus sealed tube (MFST) source or rotating anodes. All Rigaku Oxford Diffraction sources for macromolecular crystallography feature a confocal optic that is carefully selected for your source type and scientific application. Additionally, our rotating anodes are available as either single wavelength or dual wavelength (DW) to operate at two different energies.

Detector name	Active area	Readout times
PILATUS3 R 200K	83.8 mm x 70 mm	7 msec
PILATUS3 R 300K	83.8 mm x 106.5 mm	7 msec
PILATUS3 R 1M	168.7 mm x 179.4 mm	7 msec
EIGER R 1M	77.2 mm x 79.9 mm	Continuous readout, 4 µs deadtime
EIGER R 4M	155.2 mm x 162.5 mm	Continuous readout, 4 µs deadtime
HyPix-6000	77.5 mm x 80.3 mm	3.7 msec



# XtaLAB series

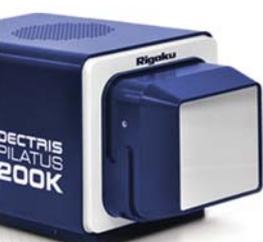
The XtaLAB platform includes a  $\frac{1}{4}$   $\chi$  goniometer along with your choice of X-ray generator, optic, and detector that best meets the needs of your lab. X-ray sources range from the low-maintenance microfocus sealed tube technology (MicroMax-003) to our high-flux microfocus rotating anode technology with proven reliability (MicroMax-007 HF and FR-X generators).

## THE XTALAB MM003

The XtaLAB MM003 system is based on the MicroMax-003 microfocus sealed tube generator and is designed for productive, low-maintenance research in your own lab. The MicroMax-003 is the perfect X-ray source for labs that want the benefit of a microfocus X-ray source with low power consumption and long tube life without the added maintenance that goes with a more powerful rotating anode generator.

### Benefits of the XtaLAB MM003 system

- Low maintenance source with superior beam stability
- Small footprint for easy integration into any lab space.
- Small beam size that is optimized for small crystals
- Extremely low noise detector allows better measurement of weak data
- Ideal system for sample screening prior to synchrotron trips and routine data collection for many samples



The XtaLAB MM003 system

### FEATURES

- Microfocus sealed tube copper X-ray source with confocal double-bounce optics
- PILATUS3 R 200K detector with true shutterless data collection capabilities
- HKL-3000R<sup>®</sup> for instrument control, data processing and structure solution—includes the world's most frequently cited data processing package, HKL-2000<sup>®</sup>, and utilizes a finely tuned structure solution pipeline based on the experience gained from high-throughput structural genomics projects.

The MicroMax-003 is configured with a specially designed confocal Max-Flux<sup>®</sup> multilayer optic. This double-bounce optic provides up to 70 times better Cu  $K\beta$  suppression compared to single bounce optics, as well as lower divergence and higher intensity. When coupled with the highly sensitive PILATUS3 R 200K detector, the MicroMax-003 gives you a great tool for both screening and structure solution.

# MicroMax-007 HF

## ROTATING ANODE X-RAY SYSTEMS

For macromolecular samples that require higher intensity sources, Rigaku Oxford Diffraction offers two options: the MicroMax-007 HF and the FR-X. Both offer the smallest available focal spot size with a patented 70  $\mu\text{m}$  beam size on the anode. Rigaku Oxford Diffraction offers the only rotating anode generator with a focal spot size below 0.1 mm, making them true microfocus generators.

## THE XTALAB MM007-HF

The XtaLAB MM007-HF system includes the MicroMax-007 HF which provides the best balance between outstanding performance for a wide range of crystal types and maximum uptime with long maintenance intervals. Moreover, maintenance procedures such as filament exchanges are quick and painless. The MicroMax-007 HF rotating anode generator offers two ports and can be equipped with detector systems on each. Alternatively, one port can be configured for biological SAXS experiments.



The MicroMax-007 X-ray source

## FEATURES OF THE XTALAB MM007-HF AND XTALAB FR-X SYSTEMS

- True microfocus rotating anode X-ray sources with outstanding beam stability
- Increased uptime and ease of use with pre-aligned and pre-aged filaments
- Your choice of VariMax™ confocal double-bounce optics for better spectral purity and beam size to match your sample types
- Four-circle goniometer to provide completeness and redundancy for your data sets
- HPC detector with true shutterless data collection capabilities
- HKL-3000R for instrument control, data processing and structure solution
- The FR-X has the added feature of 2.5 X higher flux compared to the MicroMax-007 HF

# FR-X

The FR-X  
rotating anode generator



## FR-X

The XtaLAB FR-X system includes the FR-X rotating anode generator. The FR-X is the most intense home lab X-ray source in the world and enables data collection on the widest range of protein crystal samples. It delivers 2.5 times higher flux compared to the MicroMax-007 HF rotating anode generator but shares the same microfocus 70  $\mu\text{m}$  focal spot size.

When coupled with Rigaku's VariMax optics, the FR-X delivers the highest brilliance for any commercially available rotating anode. As a result, it is possible to collect diffraction data for samples where no diffraction can be seen using a conventional rotating anode or sealed tube source.

The FR-X also offers two X-ray ports and optional dual wavelength capabilities. When using both ports, there is no compromise in beam intensity for either port.

### Benefits of the XtaLAB MM007-HF and XtaLAB FR-X systems

- Outstanding, proven reliability – X-ray generators designed with maximum uptime in mind
- Robust direct-drive anode provides extended anode and filament lifetimes
- Dual ports allow for dual detectors or dual crystallography and SAXS ports, with NO compromise in beam intensity
- Dual wavelength option – for in-house phasing or dual macro- and small molecule capabilities
- Extremely low noise detector allows for better measurement of weak data

# *in-situ* crystallography

## XTALCHECK

Protein crystallography often requires screening large numbers of crystals to identify samples that are suitable for X-ray diffraction experiments. Specifically, crystallographers usually loop and cryocool samples for X-ray screening to identify whether the sample contains a protein or salt and to evaluate diffraction resolution, mosaicity and other crystal parameters. This iterative process of mounting and screening of many samples is time consuming and rarely automated.

The XtalCheck system addresses this bottleneck by automating diffraction data collection for crystals directly from SBS format crystallization plates. Moreover, the system was developed to use your laboratory's existing X-ray diffraction system.

### FEATURES

- Automated imaging of crystallization drops
- Easy assignment of and sizing for crystal objects
- Assign multiple crystal objects per drop
- Simple queuing of crystal objects for diffraction screening
- Database tracking of crystal and diffraction images



### Benefits of the XtalCheck

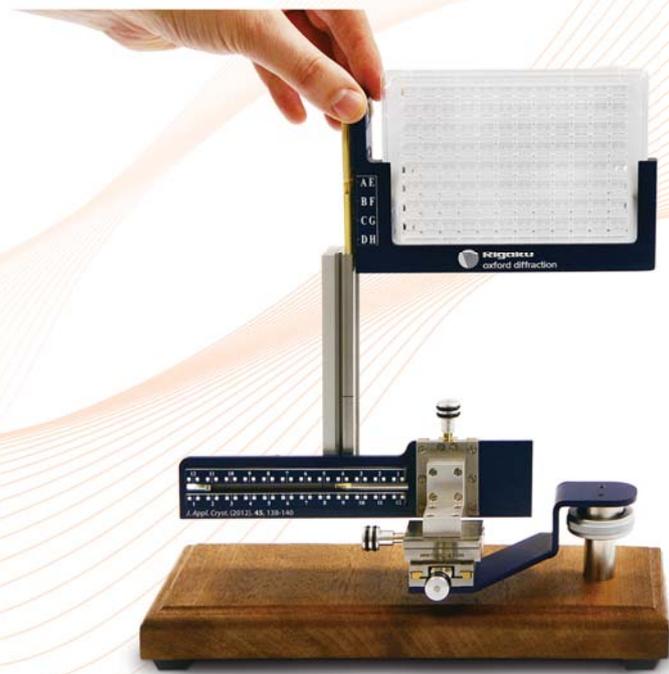
- Quickly identify and analyze samples from crystallization plates to identify salt versus protein and evaluate diffraction quality
- Automated capture of both optical and X-ray images
- Allows for automated evaluation of many crystals from many drops
- Includes a database of optical and X-ray diffraction images to allow easy review of current and past experiments
- Collect up to 40 degrees of data for a single crystal object, depending on the plate type



XtalCheck plate holder mounted on Rigaku XtaLAB MM007HF system with PILATUS3 R 200K detector

## PLATEMATE

The PlateMate is a simple, inexpensive tool for manual screening of crystals within crystallization plates. The PlateMate is a manual device that mounts onto an existing goniometer, and you use your existing X-ray source and data collection software for collecting diffraction images. This offers the advantage of using a higher intensity rotating anode for screening smaller or more weakly diffracting samples. The PlateMate supports several SBS format crystallization plates, though best results are observed using X-ray compatible plates. With the PlateMate, you can detect whether you have protein versus salt crystals within minutes. Moreover, the PlateMate has a compact design so that you can collect up to 55° of data.



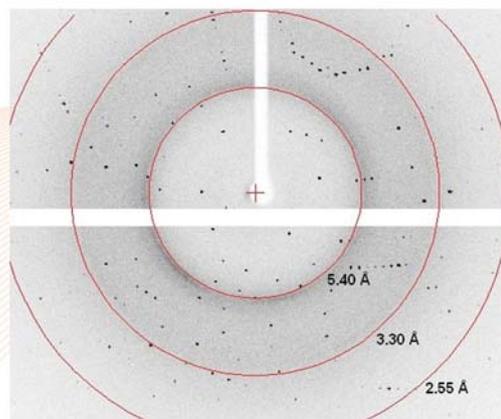
PlateMate *in-situ* screening adapter

### Benefits of the PlateMate *in-situ* screening adapter

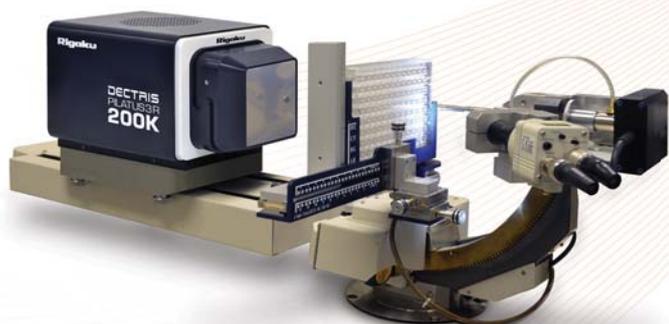
- Low cost option for *in-situ* crystallography using your existing X-ray diffraction system
- Simple, light and easy to use design
- Use your existing video system and PlateMate micrometers to center on a desired sample
- Supports most SBS format plates
- Manual design allows for greater flexibility for collecting up to 55 degrees of diffraction data

### FEATURES

- IUCr fitting allows installation with standard goniometers
- Micrometers to allow for fine plate positioning of small crystals
- Low profile design allows for collection of complete X-ray diffraction data sets for many samples



Example diffraction image collected using PlateMate installed on a MicroMax-007 HF rotating anode generator and PILATUS3 R 200K



# Small Angle X-ray Scattering

## BioSAXS-2000

Rigaku Oxford Diffraction's BioSAXS-2000<sup>1</sup> is a small angle X-ray scattering system specifically designed for isotropically scattering samples, like those found in structural biology. The BioSAXS-2000 is a modern variation of the Kratky camera that eliminates the need for data corrections due to smearing, and is capable of collecting data on most samples in 15 – 30 minutes. The BioSAXS-2000 has the advantage that it can be mounted on a variety of X-ray sources, including the open port of a rotating anode.

### FEATURES

- 2D modern Kratky system with OptiSAXS confocal optic
- Automated alignment of collimation system and beam stop
- Photodiode beamstop for intensity measurements and sample transmission corrections
- Easy to use SAXSLab software
- Uses Rigaku's HPC detector, the HyPix-3000, to deliver maximum signal to noise
- BioSAXS AUTO options include Automatic Analysis Pipeline (AAP) using the industry standard ATSAS package for automated sample analysis and the Automatic Sample Changer (ASC) that automates data collection for up to 96 samples



BioSAXS-2000 with ASC-96

### Benefits of the BioSAXS-2000

- Easily installed on the open port of an existing generator
- 2D Kratky design means higher flux on the sample without the need for data corrections due to smearing
- OptiSAXS optic offers a high X-ray capture angle to deliver outstanding flux performance and faster SAXS experiments
- Rigaku's HyPix-3000 HPC detector delivers highest sensitivity and lowest noise, making it ideal for measuring the weak scattering signal from biological solutions
- The BioSAXS AUTO package adds automated sample loading, data collection and analysis to make SAXS samples faster to perform and easier to evaluate for both novices and experts

# BioSAXS AUTO



ASC for BioSAXS-2000

## AUTOMATIC SAMPLE CHANGER

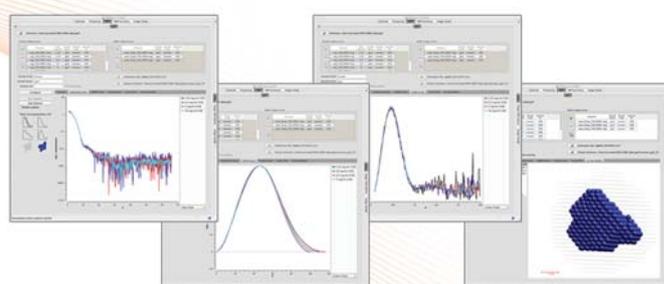
For those labs that desire unattended sample mounting and data collection, the BioSAXS-2000 includes an optional ASC. The ASC adds automated sample loading, flow cell washing and data collection capabilities to the BioSAXS-2000. It supports samples supplied in 96-well plates or 0.2 mL PCR tube arrays and seamlessly integrates with the BioSAXS-2000 system and SAXSLab software to allow easy setup of unattended or overnight experiments. This means you can focus more time where it counts, on SAXS data analysis and publication of results.

### FEATURES

- Includes flow cell, sample loading station and flow control station
- Short distance from sample storage to measurement cell for faster loading
- Supports foil-sealed samples to ensure that your samples won't evaporate prior to data collection
- Support for multiple cleaning solutions and configurable cleaning cycles
- Temperature controlled sample storage, including option for separate storage versus data collection temperatures

## AUTOMATIC ANALYSIS PIPELINE

The AAP utilizes the industry standard ATSAS package to provide automatic analyses for each sample. As a result, the AAP allows for quick evaluation of sample quality, with color-coded results so that you can easily identify well-behaving samples versus those that exhibit aggregation and concentration effects.



### FEATURES

- Automatic profile averaging, buffer subtraction and sample evaluation
- Automatic determination of the useful data range
- Automatic Guinier, Kratky and Porod analysis to determine  $R_g$ ,  $I(0)$ , molecular weight (MW) and volume of correlation ( $V_c$ )
- Automatic  $P(r)$  calculation with report of real space  $R_g$  and  $D_{max}$  and automatic envelope calculation, averaging and analysis
- PDF report generator and easy review of previous AAP runs

### Benefits of BioSAXS AUTO

- BioSAXS AUTO combines automated sample loading and data collection with the ASC and automated data analysis with the AAP to give you more time when it counts, on advanced data analysis and publication of results
- BioSAXS AUTO gives you a beamline-like experience for your SAXS experiments

# ACTOR

## ACTOR

ACTOR is a proven commercial solution for automating routine crystal screening and data collection at both synchrotron beam lines and home laboratories. Compatible with almost any goniometer and detector combination, ACTOR eliminates much of the physical handling of samples required during crystal screening and data collection. In use in over 50 home labs and synchrotrons around the world, ACTOR is a proven solution to the problem of automation of protein crystallography.

## FEATURES

- System includes 6-axis robotic arm, automated goniometer head, sample storage dewar and cryo-resistant end effector for gripping sample
- Supports ACTOR, ALS, Unipuck and ESRF sample holders
- Storage capacity up to 240 samples in 3 dewars
- Supports Hampton, MiTeGen and SPINE pins
- Laser and in dewar pin sensors detect successful mounting and return of samples to cryogenic storage dewar



The cryo-resistant ACTOR end effector is designed to eliminate turbulence during sample mounting and dismounting

## Benefits of ACTOR

- Unattended sample mounting, data collection, analysis, strategy calculation and data reduction
- ACTOR allows you to screen up to 30 samples per hour
- Integrated sample ranking and data collection strategy algorithms



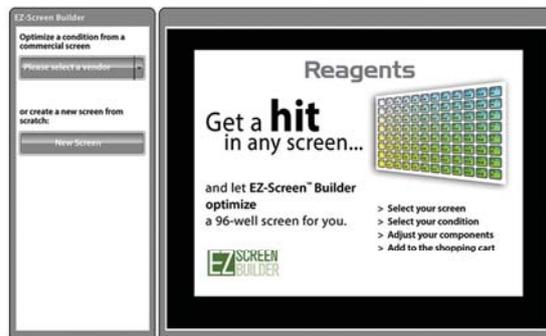
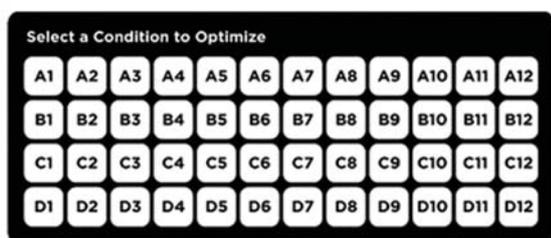
# Rigaku Reagents

## CRYSTALLIZATION SCREENS

Crystallization of proteins is challenging. No two proteins are alike and the search through crystallization space requires examining a large number of variables. Rigaku Reagents offers a broad range of screens to give you the highest probability of crystallizing your proteins of interest. For example, many labs worldwide use the Wizard Classic suite for screening crystallization conditions of proteins, peptides, and nucleic acids. Other screens include the JCSG and JCSG+ screens, which are based on those conditions that produced the highest hit rates among 500,000 crystallization trials conducted at the Joint Center for Structural Genomics. Other screens, such as the TIME and Wizard Cubic LCP kits, target the needs of membrane proteins to help identify ideal detergent conditions and explore LCP techniques.



### Wizard:Classic 1



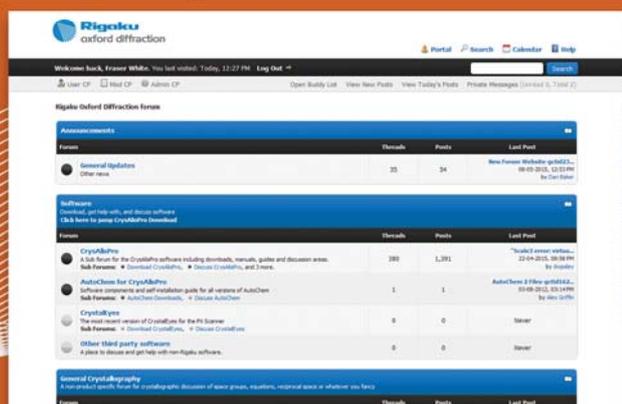
## OPTIMIZATION MADE EASY

When initial screening produces small crystals or just promising hits, optimization around these conditions becomes necessary by adjusting the various parameters from initial crystallization trials. For example, one might vary salt or precipitant concentration, pH, biomolecule concentration, or use additives. Rigaku Reagent's EZ-Screen Builder is an online tool that allows you to easily design a custom optimization screen around any hit.

Simply select the manufacturer and crystallization screen name and then your condition. You can adjust or add components before adding the screen to your shopping cart.

JOIN IN THE DISCUSSION ON THE FORUM AND NEWSLETTER

[www.rigakuxrayforum.com](http://www.rigakuxrayforum.com)



[www.rigakucrystallographytimes.com](http://www.rigakucrystallographytimes.com)



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**Your Success  
is Our Focus**

The employees of Rigaku Oxford Diffraction are dedicated to providing the best solutions for single crystal analysis, whether it be small molecule or macromolecule related research. Our inspiration comes from helping you solve your difficult experimental problems and our personal satisfaction derives from helping you achieve your research goals.

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