Application Note PX029

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# PX029 - Introducing the XtaLAB Synergy Flow

## Abstract

The XtaLAB Synergy Flow turns any XtaLAB Synergy cabinet diffractometer into an automated, high-throughput machine by incorporating a 6-axis UR3 Universal Robot and a 3-puck dewar. The XtaLAB Synergy Flow system can automatically screen and collect 48 crystal samples with minimal human intervention. CrysAlis$^{Pro}$ [1] has been upgraded with tools to control all aspects of robotics and sample queuing. A unique X-ray safe dewar-drawer system allows loading and unloading of pucks without opening the X-ray enclosure or disturbing data collection. Ultimately, the XtaLAB Synergy Flow system is the perfect solution to allow full-time use of your diffractometer during a period when human interaction and contamination must be minimized.

## Introduction

The XtaLAB Synergy products are popular diffractometers for single crystal analysis (both small molecule and macromolecular crystallography). They are complete systems containing an X-ray source, optics, goniometer and detector, all contained within the footprint of a compact cabinet. They are available with the latest high-performance microfocus sealed tube and microfocus rotating anode sources, the PhotonJet-S and PhotonJet-R, respectively. They also are available in dual-wavelength options: two separate sealed tubes and optics or two different anode materials and a single dual-wavelength optic. The XtaLAB Synergy Flow is the newest addition to the XtaLAB Synergy lineup incorporating a 6-axis UR3 Universal Robot, an X-ray safe dewar, a motorized goniometer head, and sophisticated software enhancements to CrysAlis$^{Pro}$. The XtaLAB Synergy Flow can be configured with the XtaLAB Synergy-S, XtaLAB Synergy-R, and XtaLAB Synergy-DW models, converting them into automated high-throughput machines to maximize productivity.

## UR3 robot

The XtaLAB Synergy Flow incorporates a Universal Robots UR3 6-axis robot arm mounted on the same stable base as the goniometer on the left side of the XtaLAB Synergy cabinet. A custom end effector is added to the robot for easy sample pin pickup and release while providing a protective, cryo-cooled environment for crystals during transfer. The robot has position repeatability of ± 0.1 mm at all joints to eliminate any worry of dropping pins or collisions. When the robot is not in use, it tucks itself away in the left side of the XtaLAB Synergy cabinet so the full goniometer is still accessible by the user.

**Figure 1**: Robot in the mounting position (top) and in the idle position (bottom).

## Dewar-drawer system

The XtaLAB Synergy Flow features an X-ray safe dewar-drawer system. The dewar holds up to 3 Unipucks, which is up to 48 samples. The dewar opens outside of the XtaLAB Synergy Flow X-ray enclosure. Pucks can be added or removed at any time the robot is not actively mounting or dismounting crystals. That means a crystal screening or data collection is not interrupted to access the dewar to exchange pucks. In addition, the dewar has a bar code reader, a defrost system, a rotating lid, and a liquid nitrogen level sensing system.

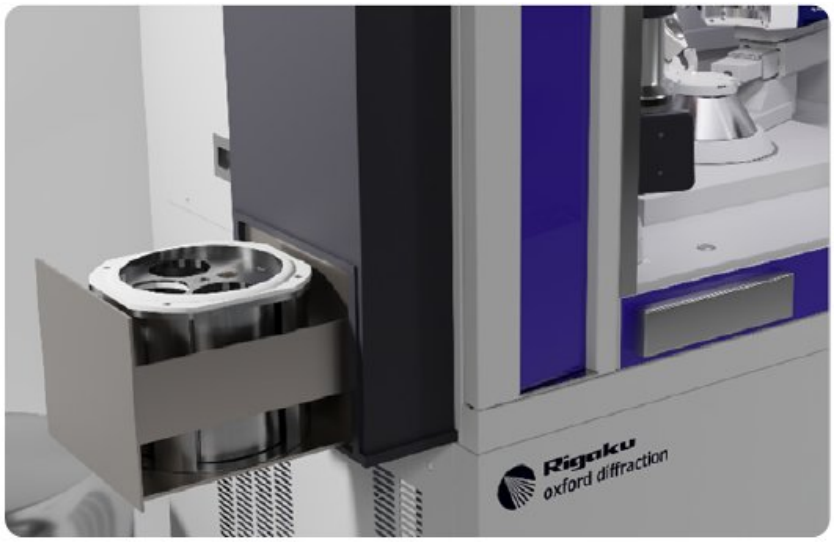


**Figure 2**: The XtaLAB Synergy Flow dewar opens by sliding out of the left side of the X-ray enclosure like a drawer.

## Intelligent Goniometer Head 2

The XtaLAB Synergy Flow features the Intelligent Goniometer Head 2 (IGH2). The IGH2 is the smallest detachable motorized goniometer head available for home lab diffractometers. It has a magnetic mount compatible with commonly used mount standards including SPINE and ALS. It works in conjunction with sophisticated image processing in CrysAlis$^{Pro}$ for auto-centering loops and crystals within the loops. In addition, manual fine tuning of centering is via point and click centering.

**Figure 3**: The IGH2 is a compact motorized goniometer head for automated crystal centering.

## CrysAlis$^{Pro}$ Robtics

CrysAlis$^{Pro}$ has been enhanced with a module called CAP Robotics to handle all aspects of robot operation, sample queuing, workflows, automatic sample centering, and presenting tables of results. Using CAP Robotics, the XtaLAB Synergy Flow can run in a fully automatic mode, a fully manual mode, or anywhere in between.

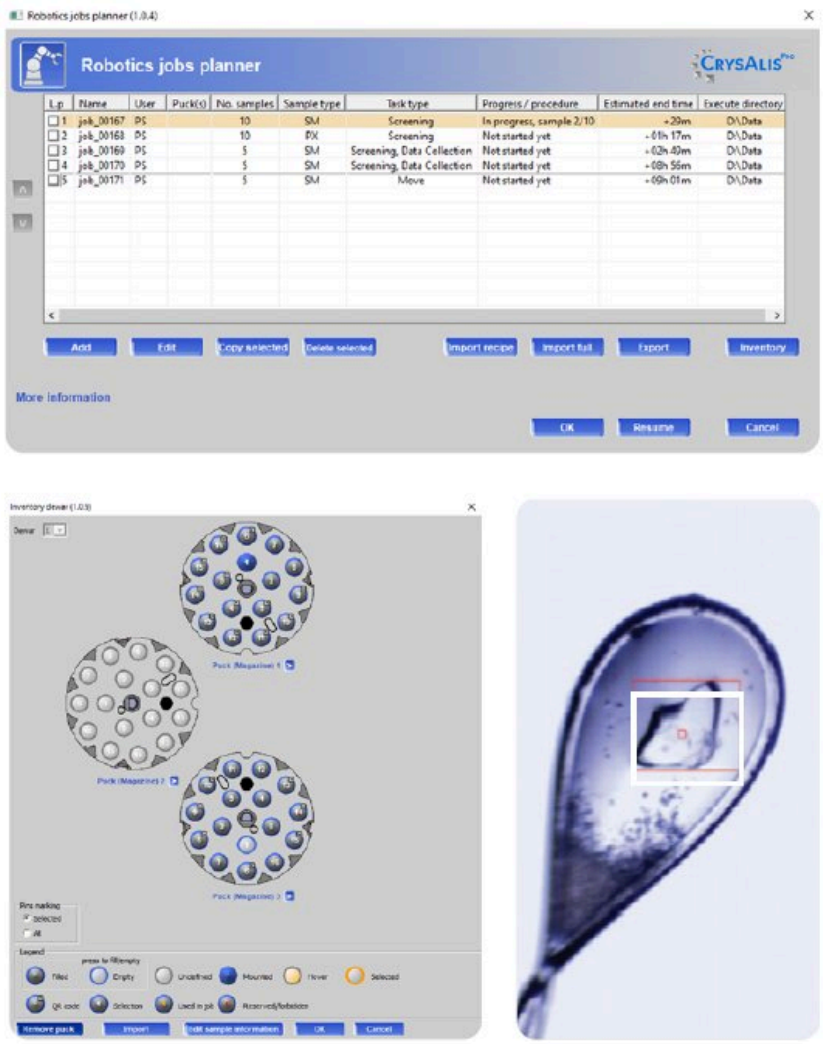


**Figure 4**: Job planner (top), dewar inventory (left) and automatic crystal centering (right).

## XtaLAB Synergy Flow results

To demonstrate an automated screening experiment with the XtaLAB Synergy Flow, eight lysozyme and eight thaumatin crystals were flash-cooled in liquid nitrogen, loaded into a Unipuck, and placed in the dewar of the instrument. A job was created to screen and rank (score the diffraction of) all the samples. The total job time from start to finish was 88 minutes, which works out to 5.5 minutes per sample. Of the 5.5 minutes, 1 m 20 s was exposure time (8 diffraction images were recorded for each sample using 10 second exposures).

Upon inspection of the Results Viewer, it was immediately clear that four out of the eight lysozyme crystals had low rank scores (<110) and incorrect unit cell parameters, and inspection of the images from crystal centering revealed no crystals in the loops. This was likely due to user error during the crystal looping and flash-cooling process. The remaining lysozyme crystals had higher scores (>400) and correct unit cells. These crystals were candidates for full data collections. All eight thaumatin crystals were present in their loops with rank scores ranging from 306 to 355 and correct unit cell parameters. All were suitable candidates for full data collections.

**Table 1**: XtaLAB Synergy Flow specifications

| | |
|---|---|
| X-ray source | PhotonJet-DW |
| Operating power | 40 kV x 30 mA = 1.2 kW |
| Optic | DW VHF Cu Mo |
| Wavelength | 1.5418 Å Cu |
| Cryosystem | Oxford Cryosystems Cobra |
| Goniometer | 4-circle Kappa with telescoping 2θ arm / distance range 47–210 mm |
| Detector | Hypix-Arc 100o |
| • Active area | 77.5 mm x 121.8 mm |
| • Frame rate | Up to 100 Hz |
| • Pixel size | 100 µm x 100 µm |
| • Cooling | Water |

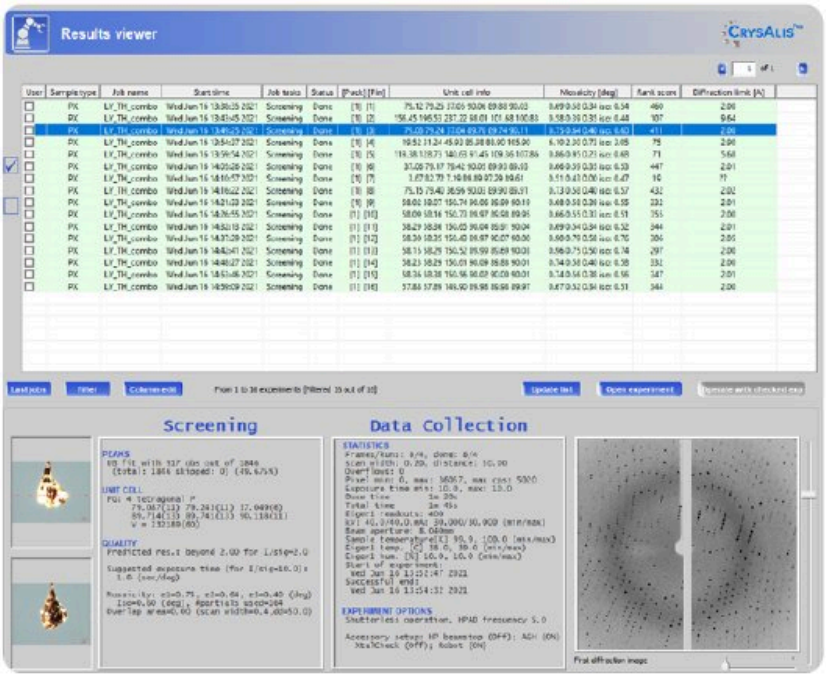


**Figure 5**: CAP Results Viewer showing a summary of the crystal screening results for lysozyme and thaumatin crystals.

## Summary

The XtaLAB Synergy Flow is the newest addition to the XtaLAB Synergy family. It can be used by both small molecule and macromolecular crystallographers. It adds auto-mounting, auto-centering, and auto-data collection to the XtaLAB Synergy platform via a robotic arm, dewar-drawer system, motorized goniometer head, and advanced software tools. The XtaLAB Synergy Flow enables unattended data acquisition, enhanced productivity, and a standardized workflow in the home laboratory.

## Reference

1. Rigaku Oxford Diffraction. (2019). CrysAlis$^{Pro}$ Software system, version 1.171.41.76a.

## Related products

### Intelligent Goniometer Head 2 (IGH2)

The smallest detachable motorized goniometer head on the market.

### XtaLAB Synergy Flow

Robotic sample changer to provide unattended data acquisi tion, enhanced productivity and standardized workflow to y our research environment.