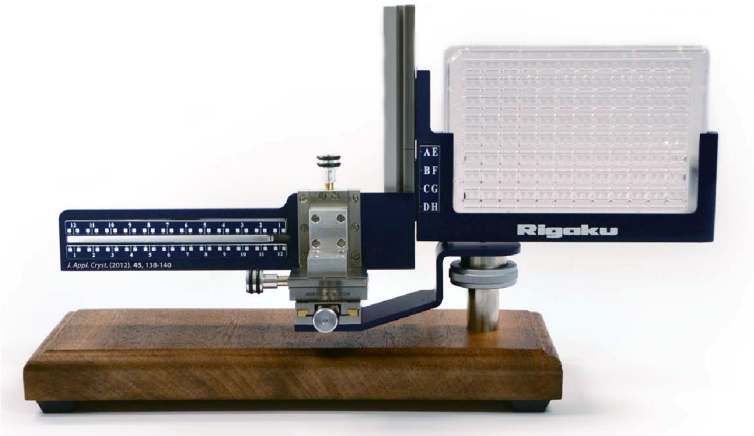
Plate adapter for *in situ* X-ray diffraction experiments

PlateMate



1. Introduction

The Rigaku PlateMate is a tool that allows one to mount SBS format crystallization plates on Rigaku goniometers for *in situ* diffraction experiments. Protein crystallography often requires screening large numbers of crystals to identify samples suitable for X-ray data collection. Traditionally, crystallographers mounted crystalline samples in capillaries — a time consuming task often resulting in damaged crystals — to evaluate sample quality prior to cryo-freezing. The PlateMate, a tool originally designed by crystallographers at AstraZeneca[1] and adapted by Rigaku, streamlines the screening process because it eliminates the need to harvest crystals from crystallization plates. Instead, crystals can be evaluated *in situ*, using existing X-ray diffraction equipment, to determine whether they are composed of protein or salt and to evaluate diffraction resolution, mosaicity and other crystal parameters. Thus, the PlateMate is a low-invasive, fast tool for benchmarking diffraction quality prior to sample harvesting and freezing.

2. Features of the PlateMate

The PlateMate is comprised of two parts: the plate nest and the base assembly (Fig. 1). SBS format crystallization plates are held into place on the plate nest with a spring-loaded clip; the plate nest then slides onto the base assembly that has previously been mounted on a goniometer. Scales, located on the plate nest and base assembly, identify the locations of wells in the bottom of the plate (rows A–D). To screen the top four rows (rows E–H), the user must invert the crystallization plate within the plate nest.

Coarse positioning of the PlateMate is achieved by sliding the plate nest along horizontal and vertical rails

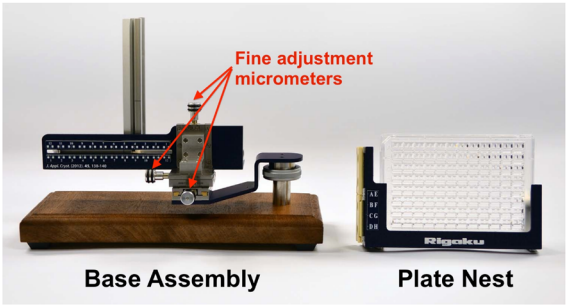


Fig. 1. The PlateMate, unassembled.

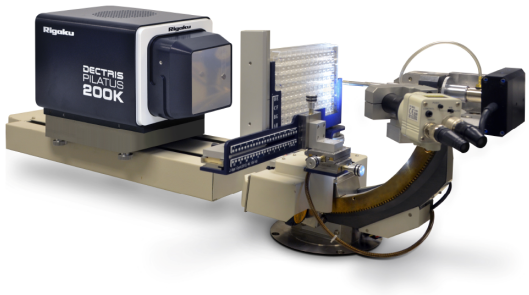


Fig. 2. PlateMate mounted on an AFC-11 goniometer configured with a PILATUS 200 K detector.

to reach the desired crystallization well. Crystals within drops are then centered in the beam with the existing camera system and fine translational adjustments along X, Y and Z with the fine adjustment micrometers located on the plate base assembly (Fig. 2). After centering the crystal in the X-ray beam, users collect diffraction data using their standard data collection package.

Other components and features of the PlateMate allow for easy screening of crystals directly from diffraction

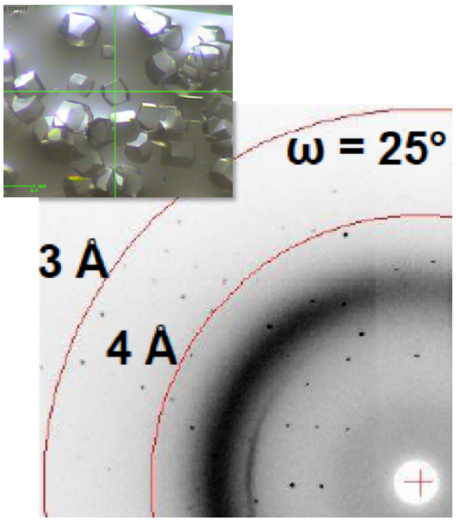


Fig. 3. Lysozyme crystal (top left) and *in situ* diffraction image (bottom right).

Table 1. Data processing results for lysozyme.

Space Group	$P4_32_12$
Unit cell	a=79.24 Å c=38.01 Å
Resolution	2.7 Å
Mosaicity	0.3–0.35°
Total reflections	11538
Unique reflections	3639
Rejected reflections	26, or 0.23%
Completeness	90.7% (79.5%)
Redundancy	3.5 (2.0)
$\langle I/\sigma(I)\rangle$	13.9 (2.8)
Linear R_{merge}	9.0% (xx%)
χ^2	1.276 (0.723)

Numbers in ( ) are for highest resolution shell.

plates. For example, the PlateMate comes with a specialized beam stop that blocks the direct beam yet allows sufficient clearance of the PlateMate hardware. The PlateMate base assembly uses a standard IUCr mount, so adapters are not required for installation on Rigaku goniometers. Finally, the easy to use PlateMate Integration module software implements collision detection and prevention so that any standard Rigaku data collection package (for example, CrystalClear, HKL-3000R® and StructureStudio) can be used. Simply double-click on the desktop icon and the module is activated. When screening or data collection with the PlateMate are complete, double-click again to switch back to data collection with standard pin mounts.

3. Typical results using the PlateMate

To test the effectiveness of screening and data collection with the PlateMate, lysozyme crystals were grown in Greiner low-profile plates. Samples of about 100 μm were then selected for data collection using the Rigaku MicroMax-007 HF configured with a Rigaku AFC-11 goniometer and Saturn 944HG CCD detector. Screen images for a 120 μm crystal, located in well E1 (Fig. 3), were collected for 10 seconds per 0.5° with a crystal-to-detector distance of 80 mm. Diffraction images showed reflections slightly beyond 3 Å (Fig. 3). For these Greiner low-profile plates, the scattering background is higher due to the plate material and excess crystallization solution. Nevertheless, images were readily indexed with HKL-3000R[(2)].

A data set with a rotation range totaling 43° was collected at room temperature using an exposure time of 20 seconds per 0.5°. The diffraction patterns showed single crystal diffraction on all images, suggesting that none of the neighboring crystals within the drop had entered the X-ray beam throughout the rotation range, despite their proximity to the target crystal. Data were processed with HKL-3000R (Table 1).

These results with lysozyme and other proteins (not shown) illustrate that the PlateMate is a capable tool for collecting diffraction data on crystals directly from crystallization plates. Moreover, the PlateMate can be used with existing X-ray diffraction hardware to expand the home lab capabilities and to provide a low-cost, low-invasive method for rapidly *in situ* screening or data collection.

References

(1) D. Hargreaves: *J. Appl. Cryst.*, **45** (2012), 138–140.
(2) W. Minor, M. Cymborowski, Z. Otwinowski and M. Chruszcz: *Acta Cryst.*, **D62** (2006), 859–866.